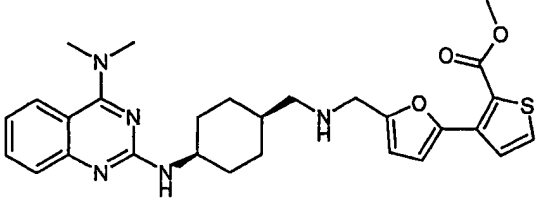
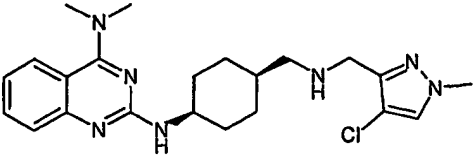
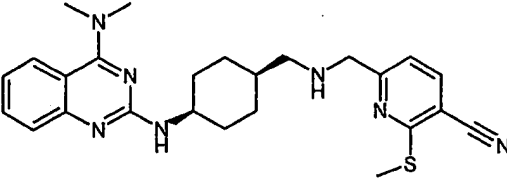
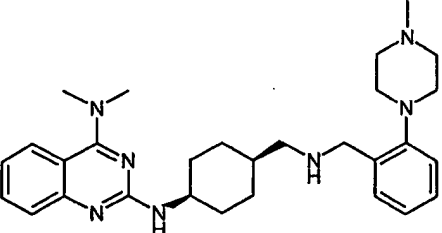
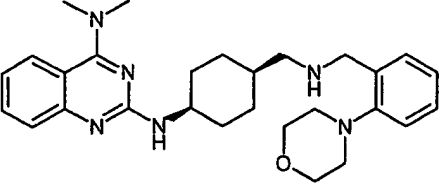
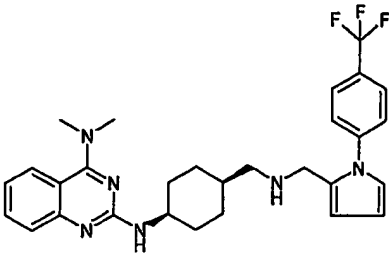
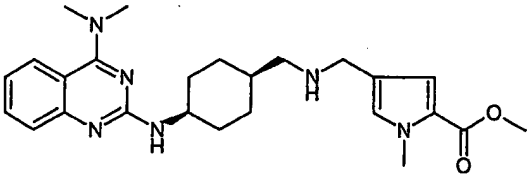
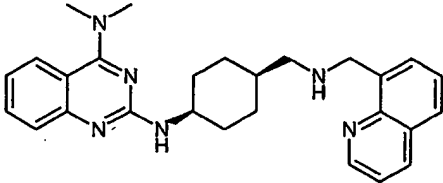
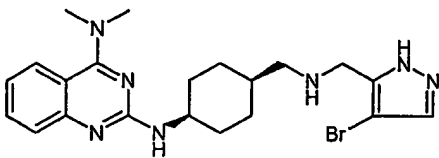
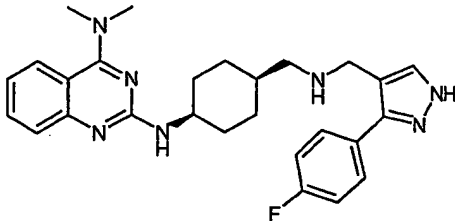
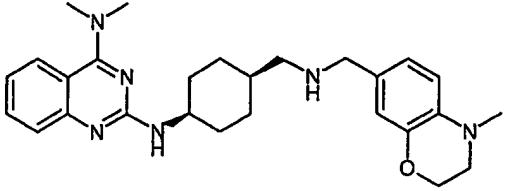
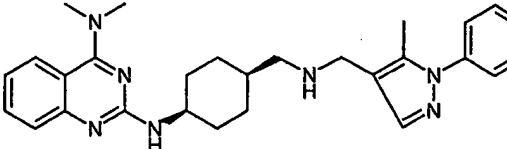
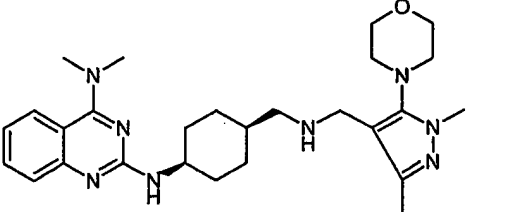
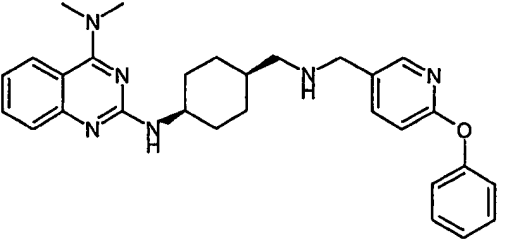
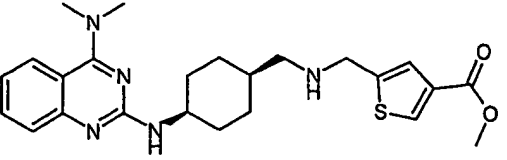
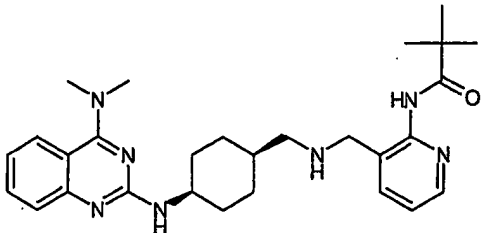
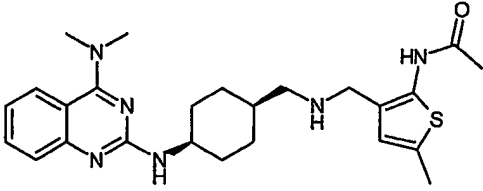
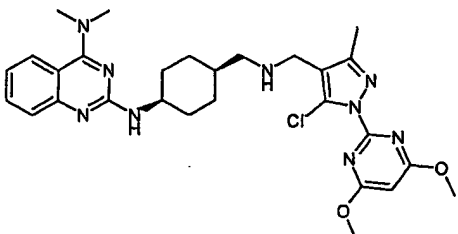
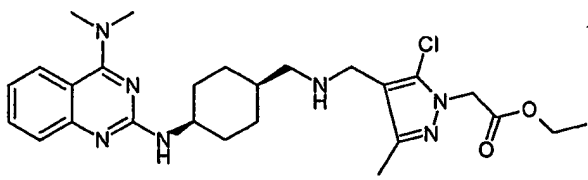
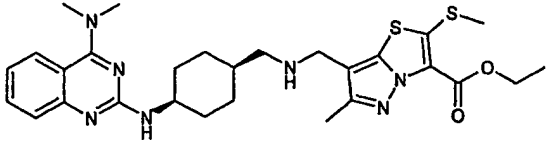
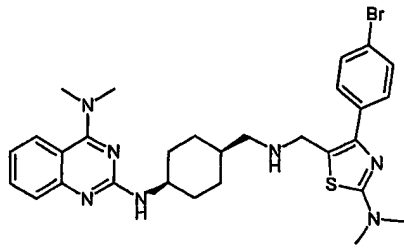
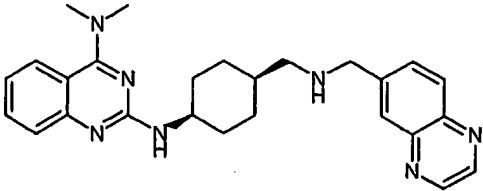
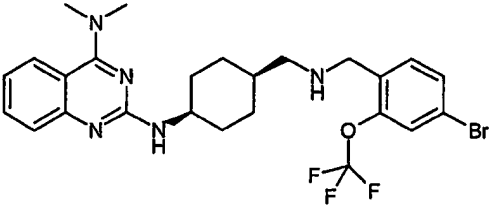
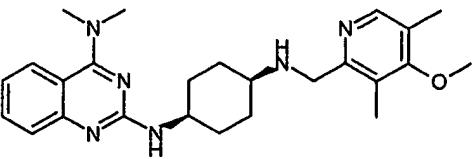
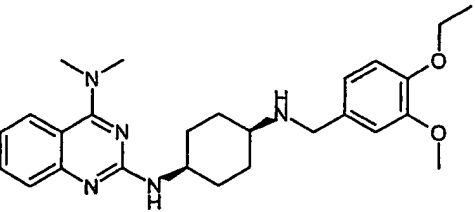


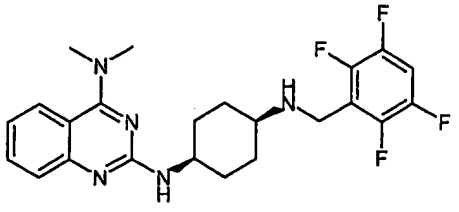
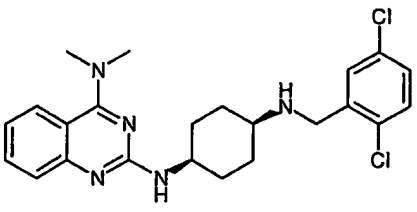
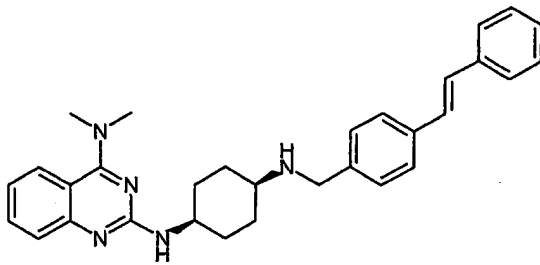
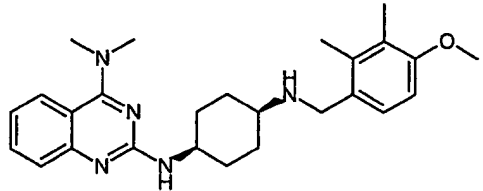
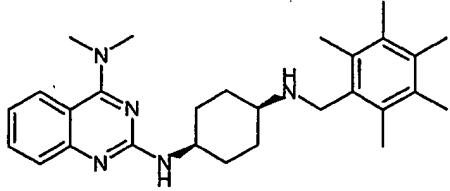
Example No.	Structure	APCI-MS
2162		520 (M + H)
2163		428 (M + H)
2164		462 (M + H)
2165		488 (M + H)
2166		475 (M + H)

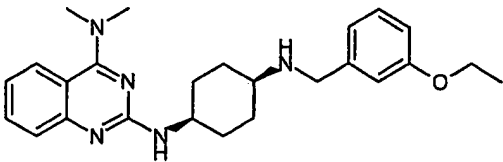
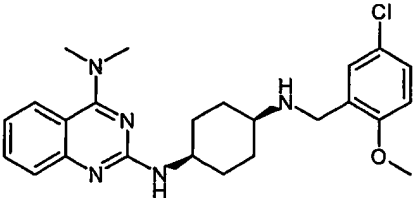
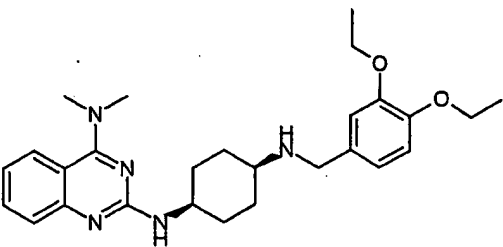
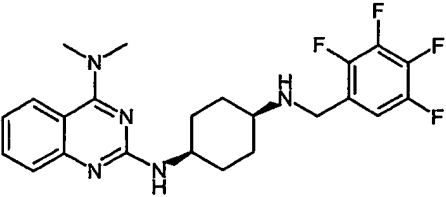
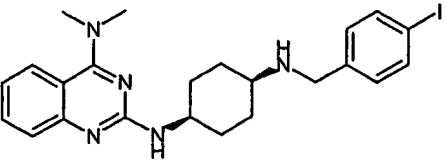
Example No.	Structure	APCI-MS
2167		523 (M + H)
2168		451 (M + H)
2169		441 (M + H)
2170		458 (M + H)
2171		474 (M + H)

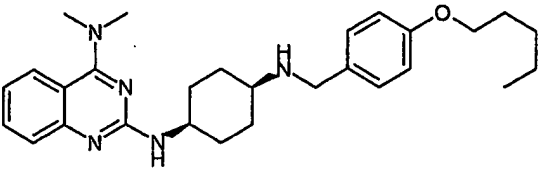
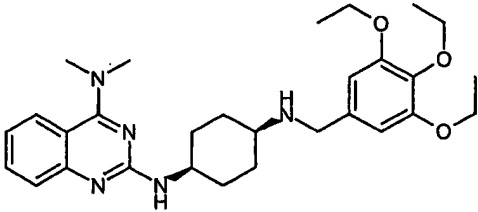
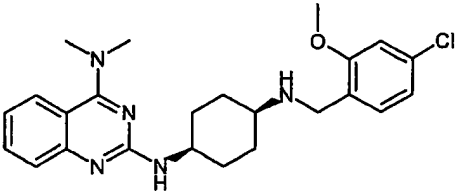
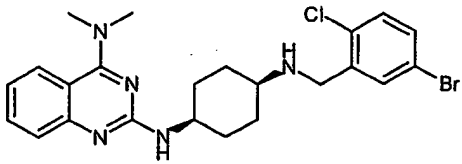
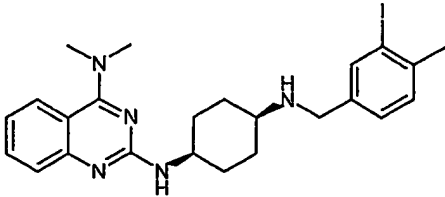
Example No.	Structure	APCI-MS
2172		461 (M + H)
2173		470 (M + H)
2174		493 (M + H)
2175		483 (M + H)
2176		454 (M + H)

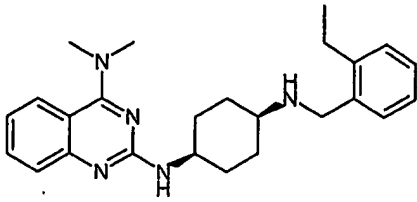
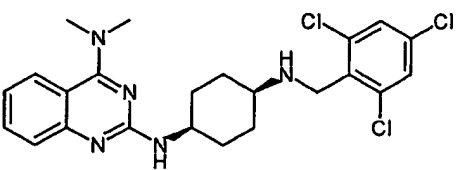
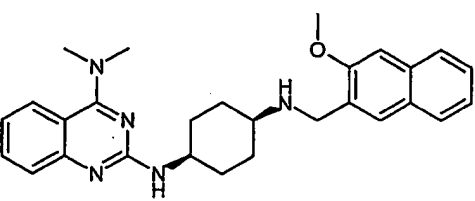
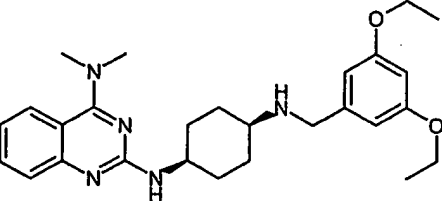
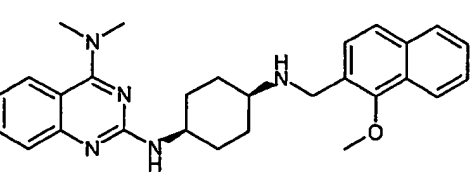
Example No.	Structure	APCI-MS
2177		490 (M + H)
2178		467 (M + H)
2179		566 (M + H)
2180		514 (M + H)
2181		568 (M + H)

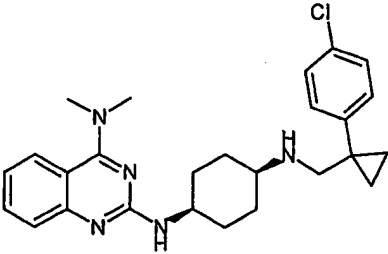
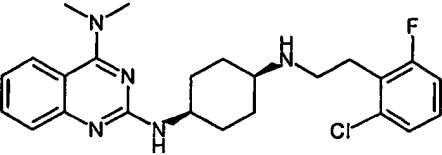
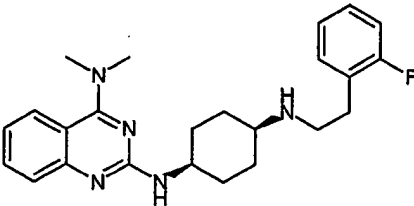
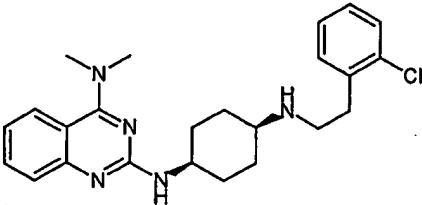
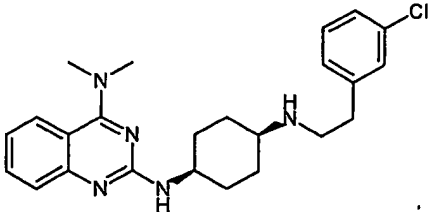
Example No.	Structure	APCI-MS
2182		594 (M + H)
2183		442 (M + H)
2184		552 (M + H)
2185		435 (M + H)
2186		450 (M + H)

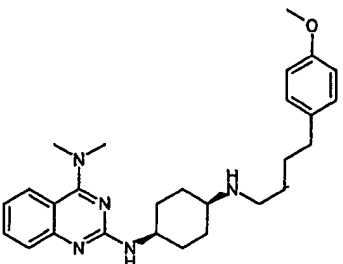
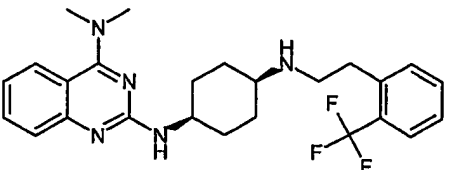
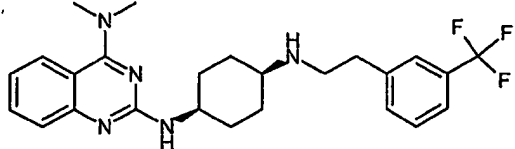
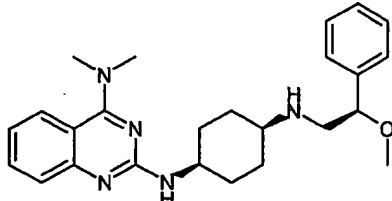
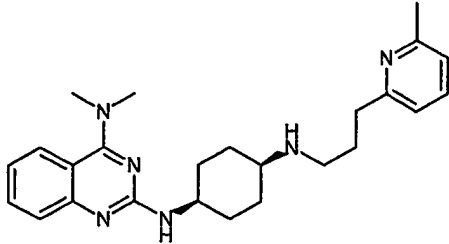
Example No.	Structure	APCI-MS
2187		448 (M + H)
2188		444 (M + H)
2189		478 (M + H)
2190		434 (M + H)
2191		446 (M + H)

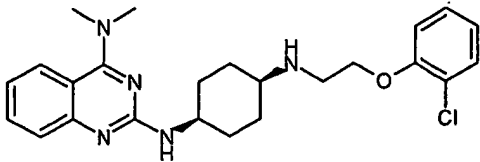
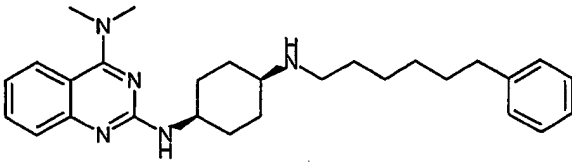
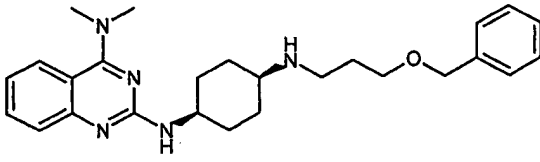
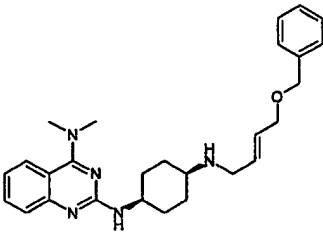
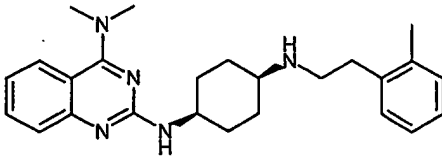
Example No.	Structure	APCI-MS
2192		420 (M + H)
2193		440 (M + H)
2194		464 (M + H)
2195		448 (M + H)
2196		502 (M + H)

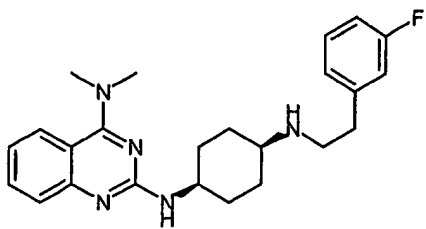
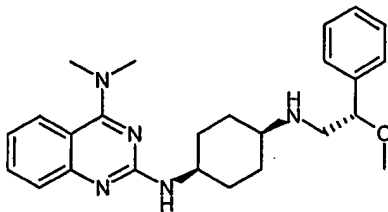
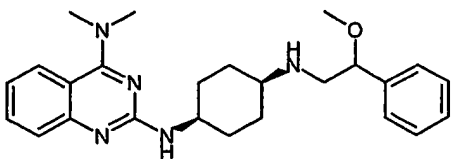
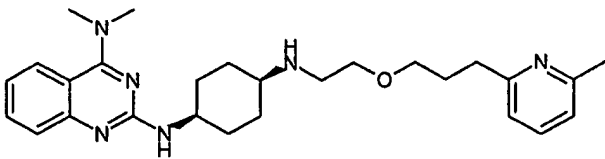
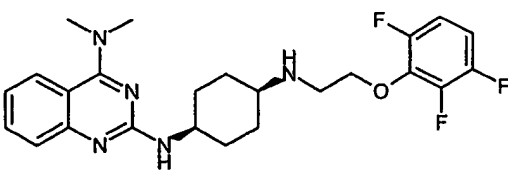
Example No.	Structure	APCI-MS
2197		462 (M + H)
2198		508 (M + H)
2199		440 (M + H)
2200		488 (M + H)
2201		516 (M + H)

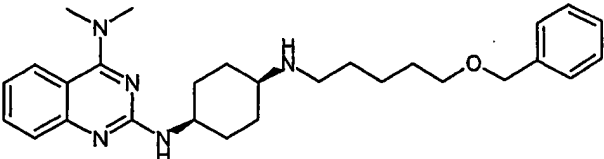
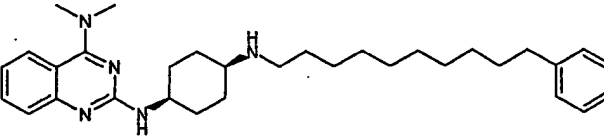
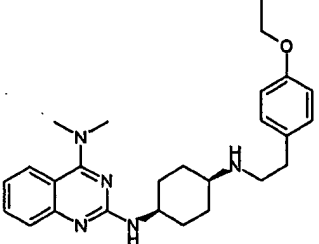
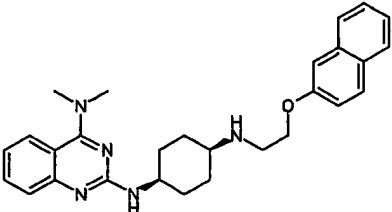
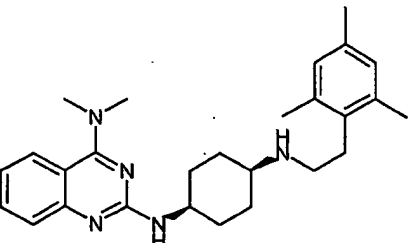
Example No.	Structure	APCI-MS
2202		404 (M + H)
2203		478 (M + H)
2204		456 (M + H)
2205		464 (M + H)
2206		456 (M + H)

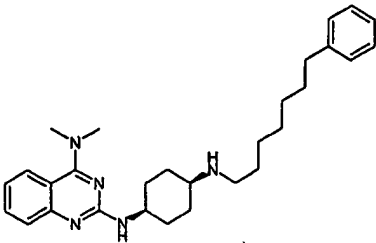
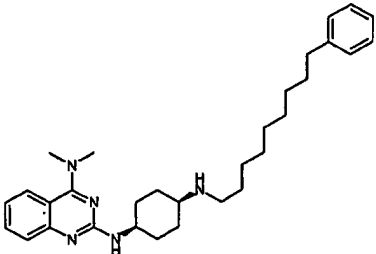
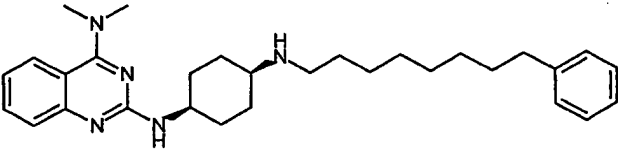
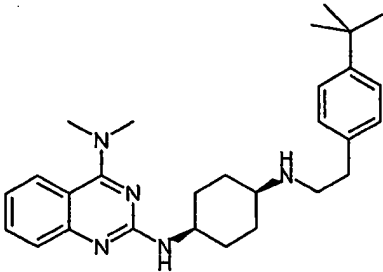
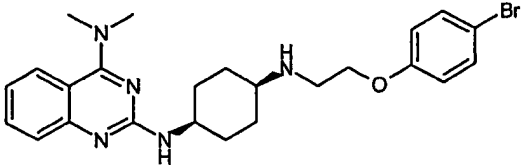
Example No.	Structure	APCI-MS
2207		450 (M + H)
2208		442 (M + H)
2209		408 (M + H)
2210		424 (M + H)
2211		424 (M + H)

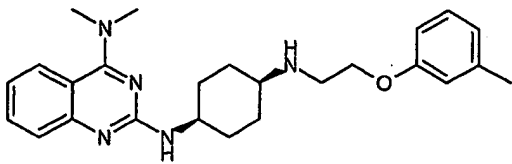
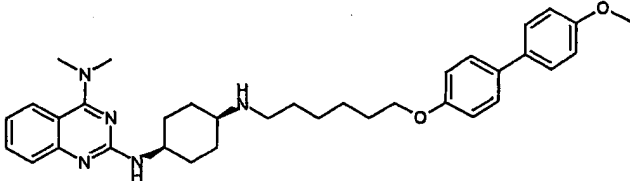
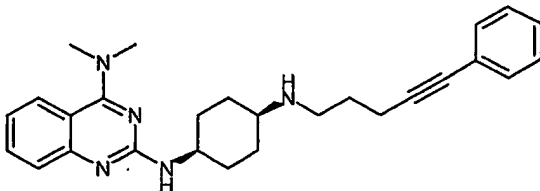
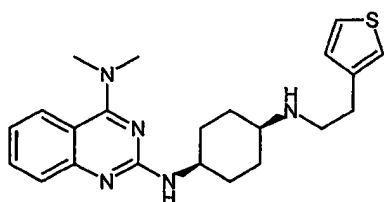
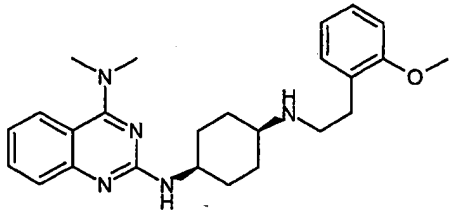
Example No.	Structure	APCI-MS
2212		448 (M + H)
2213		458 (M + H)
2214		458 (M + H)
2215		420 (M + H)
2216		419 (M + H)

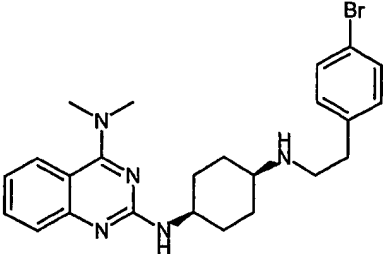
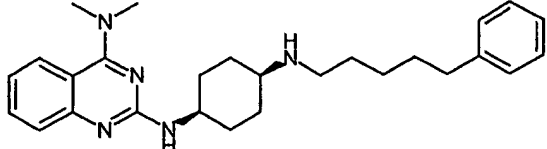
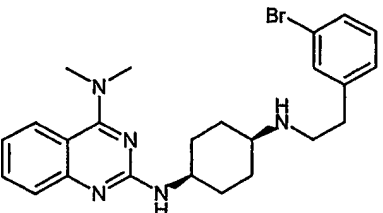
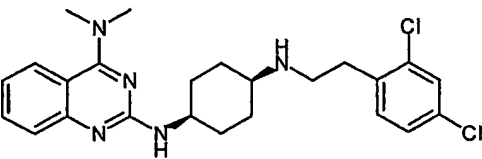
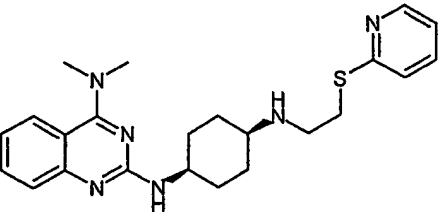
Example No.	Structure	APCI-MS
2217		440 (M + H)
2218		446 (M + H)
2219		434 (M + H)
2220		446 (M + H)
2221		404 (M + H)

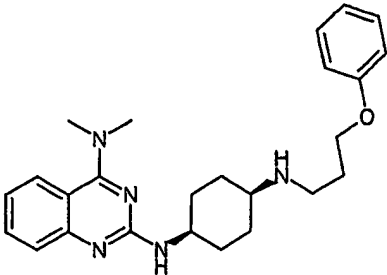
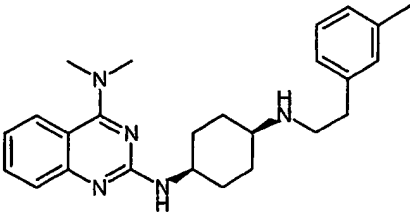
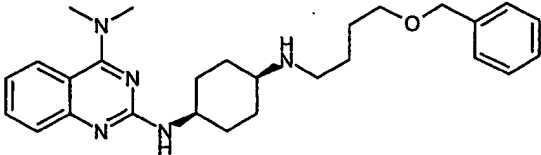
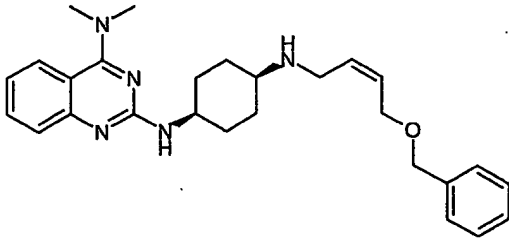
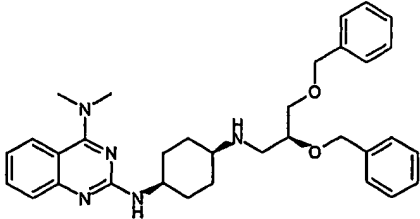
Example No.	Structure	APCI-MS
2222		408 (M + H)
2223		420 (M + H)
2224		420 (M + H)
2225		463 (M + H)
2226		460 (M + H)

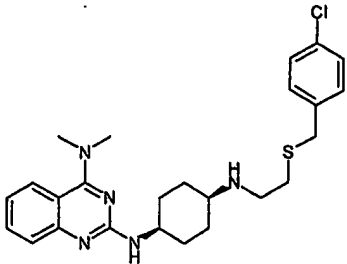
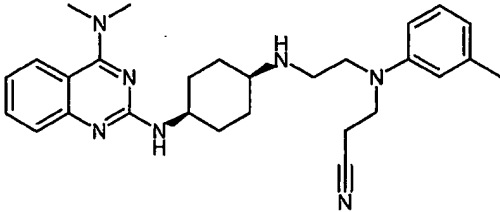
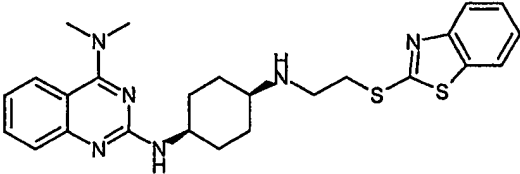
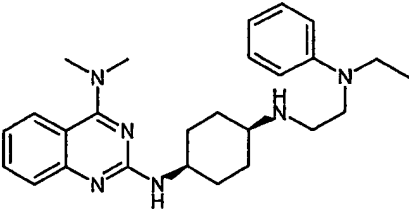
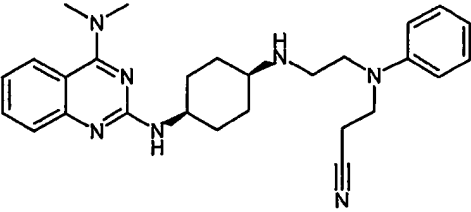
Example No.	Structure	APCI-MS
2227		462 (M + H)
2228		502 (M + H)
2229		434 (M + H)
2230		456 (M + H)
2231		432 (M + H)

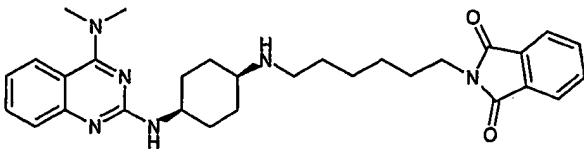
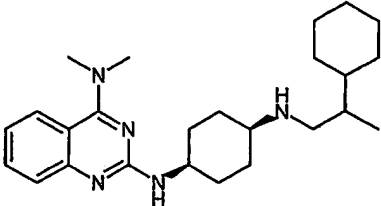
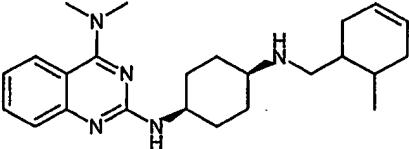
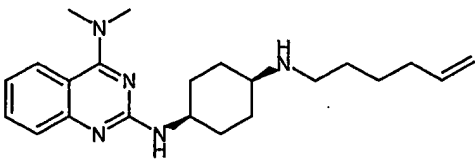
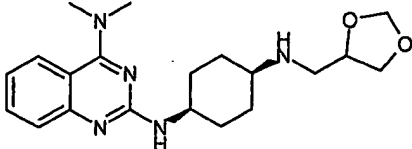
Example No.	Structure	APCI-MS
2232		460 (M + H)
2233		488 (M + H)
2234		474 (M + H)
2235		446 (M + H)
2236		484 (M + H)

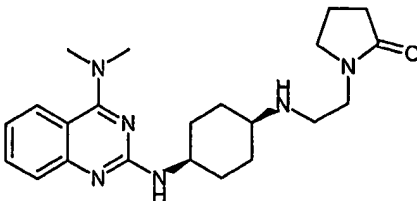
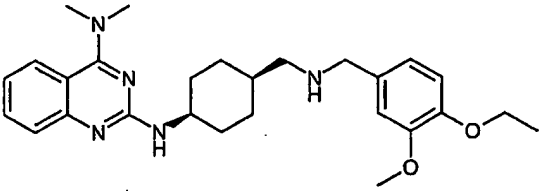
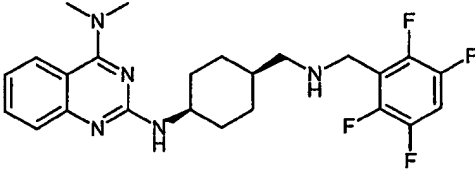
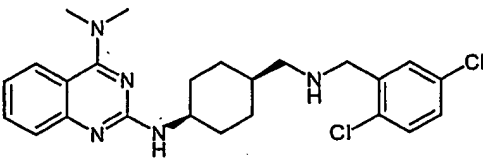
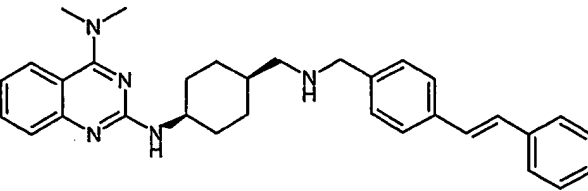
Example No.	Structure	APCI-MS
2237		420 (M + H)
2238		568 (M + H)
2239		428 (M + H)
2240		396 (M + H)
2241		420 (M + H)

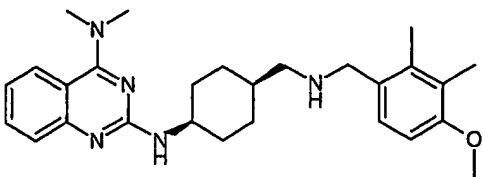
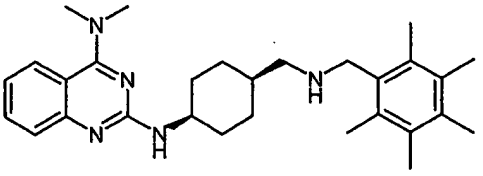
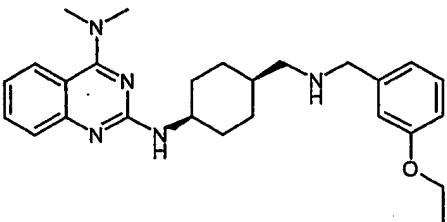
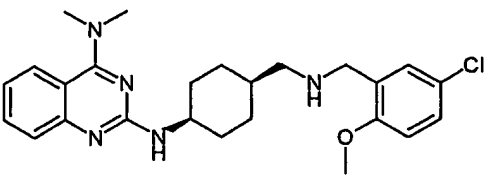
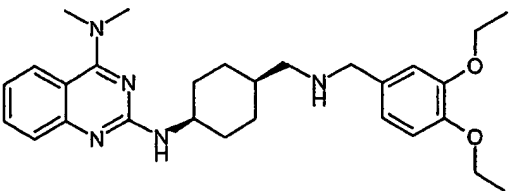
Example No.	Structure	APCI-MS
2242		468 (M + H)
2243		432 (M + H)
2244		468 (M + H)
2245		458 (M + H)
2246		423 (M + H)

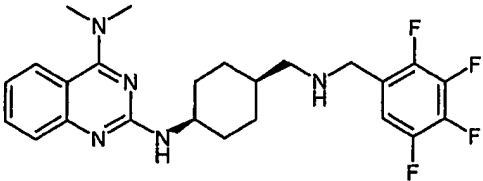
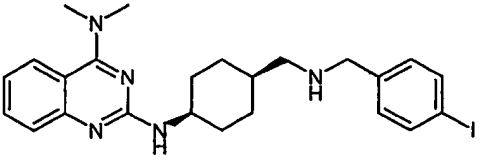
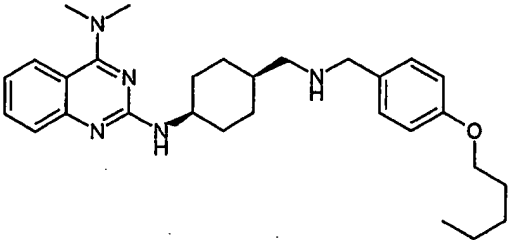
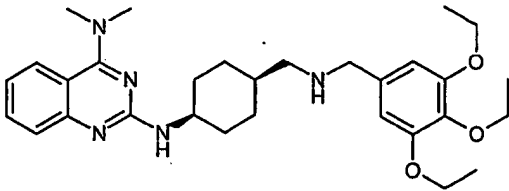
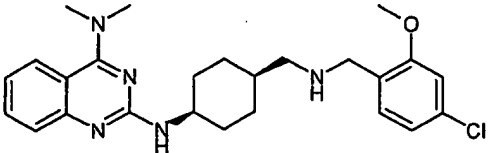
Example No.	Structure	APCI-MS
2247		420 (M + H)
2248		404 (M + H)
2249		448 (M + H)
2250		446 (M + H)
2251		540 (M + H)

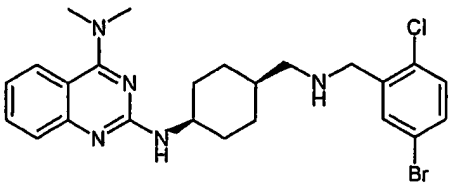
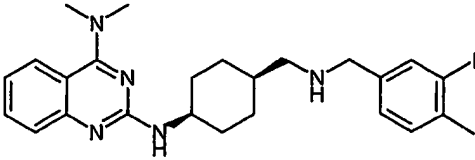
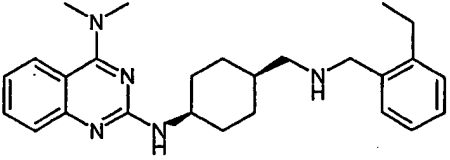
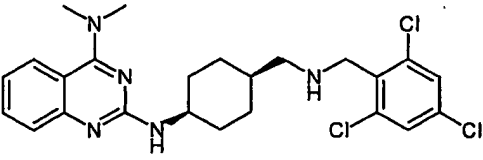
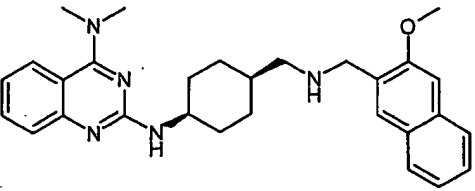
Example No.	Structure	APCI-MS
2252		470 (M + H)
2253		472 (M + H)
2254		479 (M + H)
2255		433 (M + H)
2256		458 (M + H)

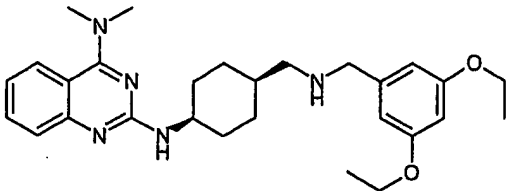
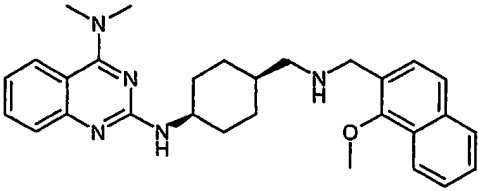
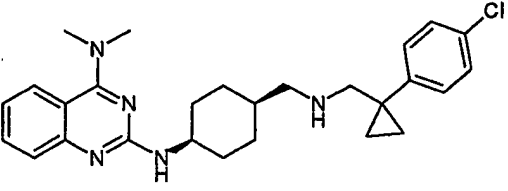
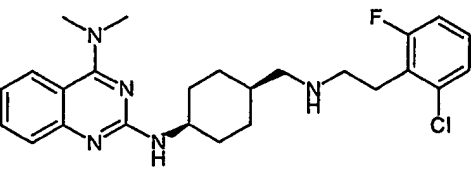
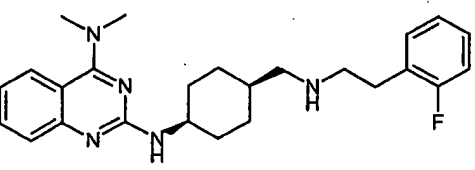
Example No.	Structure	APCI-MS
2257		515 (M + H)
2258		410 (M + H)
2259		394 (M + H)
2260		368 (M + H)
2261		372 (M + H)

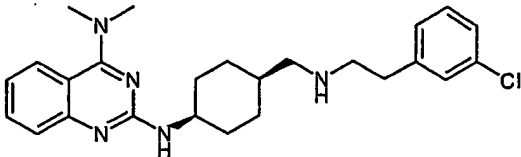
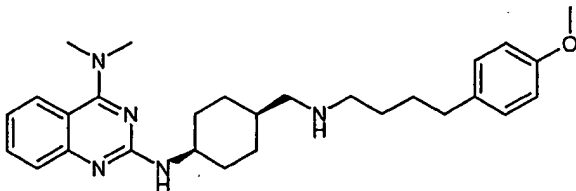
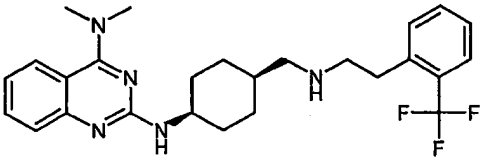
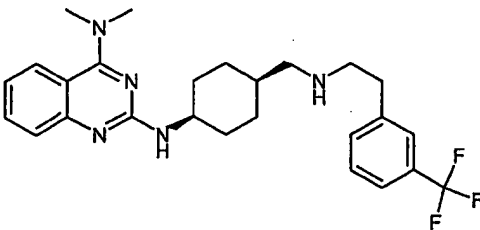
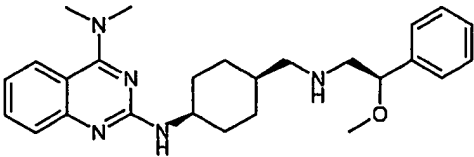
Example No.	Structure	APCI-MS
2262		397 (M + H)
2263		464 (M + H)
2264		462 (M + H)
2265		458 (M + H)
2266		492 (M + H)

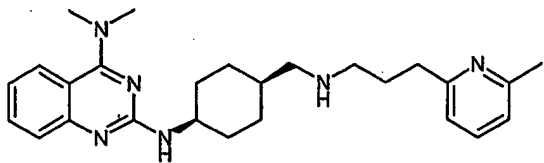
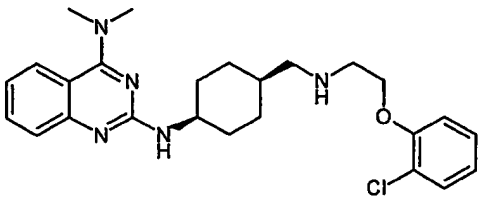
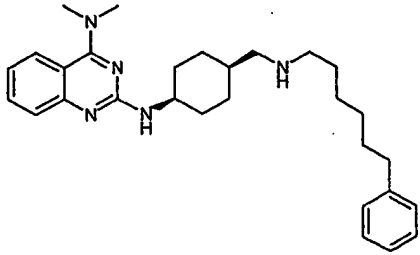
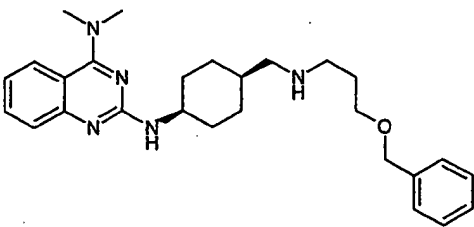
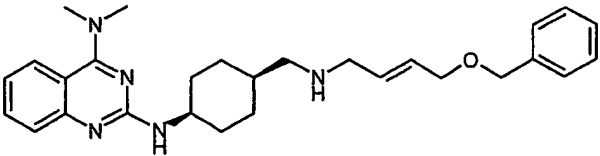
Example No.	Structure	APCI-MS
2267		448 (M + H)
2268		460 (M + H)
2269		434 (M + H)
2270		454 (M + H)
2271		478 (M + H)

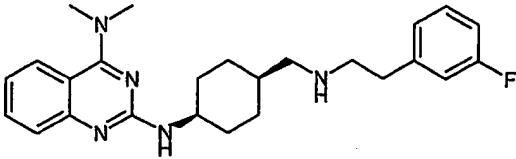
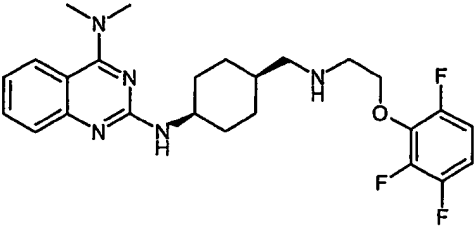
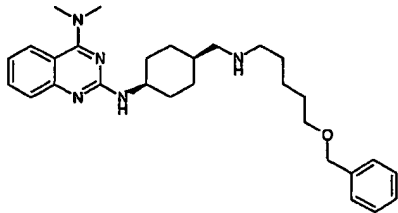
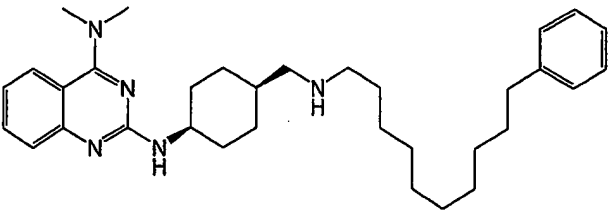
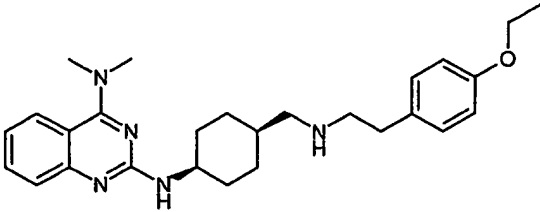
Example No.	Structure	APCI-MS
2272		462 (M + H)
2273		516 (M + H)
2274		476 (M + H)
2275		522 (M + H)
2276		454 (M + H)

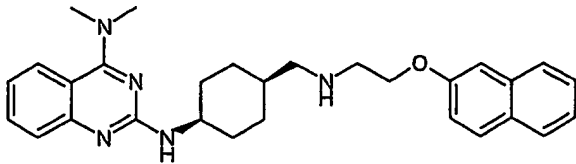
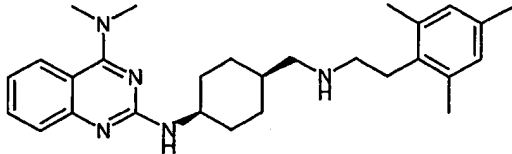
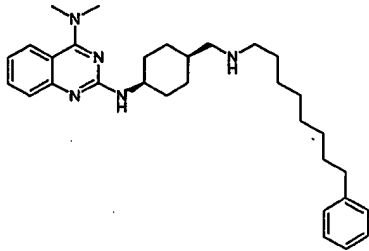
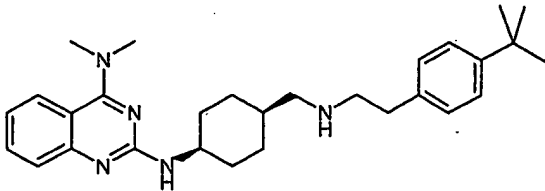
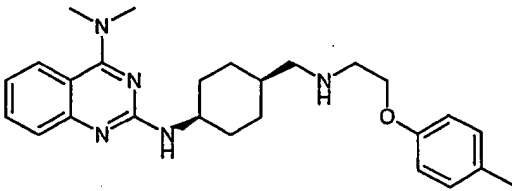
Example No.	Structure	APCI-MS
2277		502 (M + H)
2278		530 (M + H)
2279		418 (M + H)
2280		492 (M + H)
2281		470 (M + H)

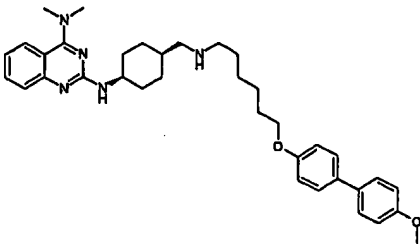
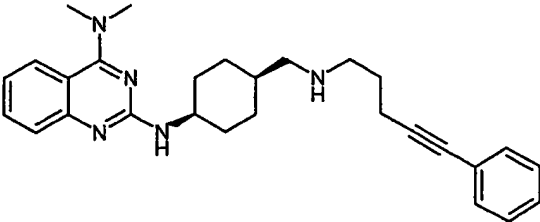
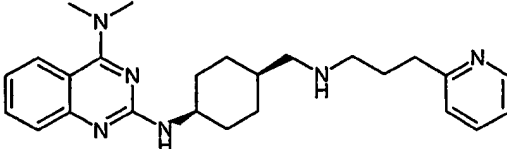
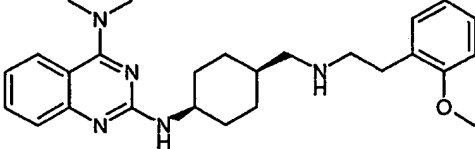
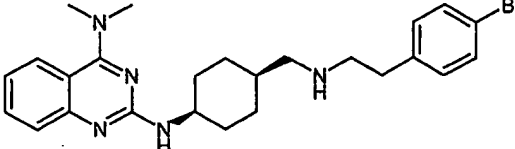
Example No.	Structure	APCI-MS
2282		478 (M + H)
2283		470 (M + H)
2284		464 (M + H)
2285		456 (M + H)
2286		422 (M + H)

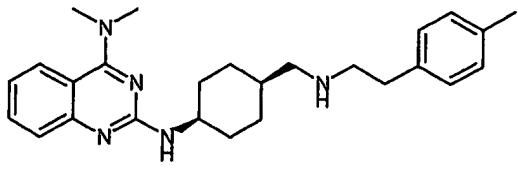
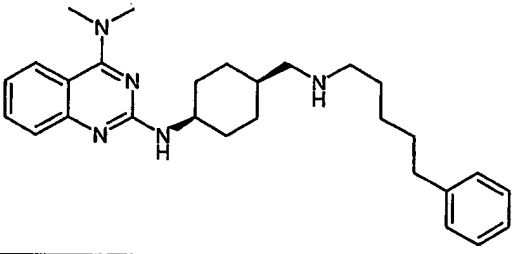
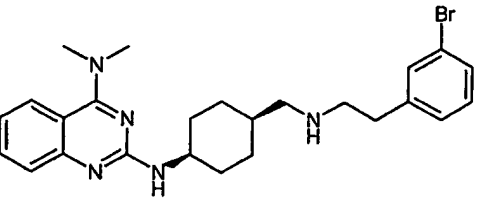
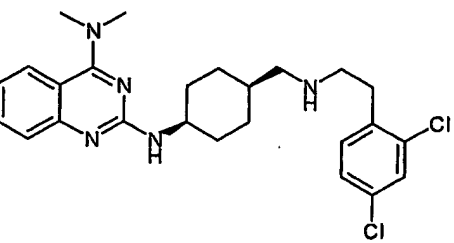
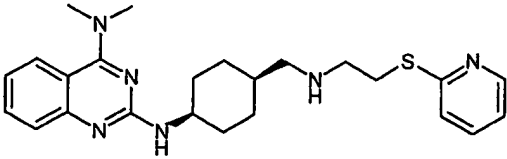
Example No.	Structure	APCI-MS
2287		438 (M + H)
2288		462 (M + H)
2289		472 (M + H)
2290		472 (M + H)
2291		434 (M + H)

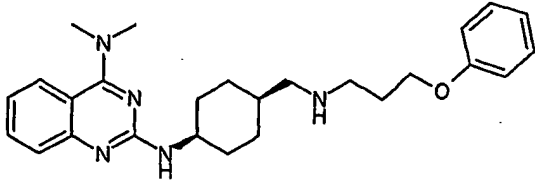
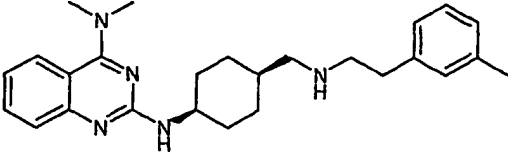
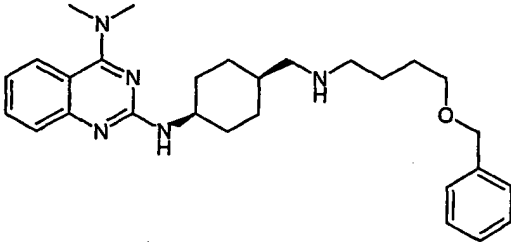
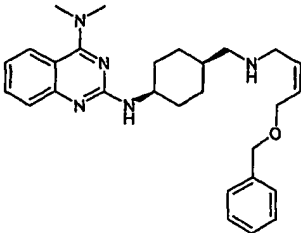
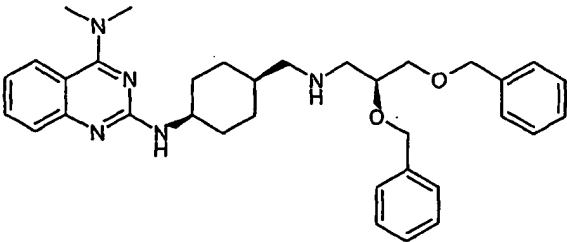
Example No.	Structure	APCI-MS
2292		433 (M + H)
2293		454 (M + H)
2294		460 (M + H)
2295		448 (M + H)
2296		460 (M + H)

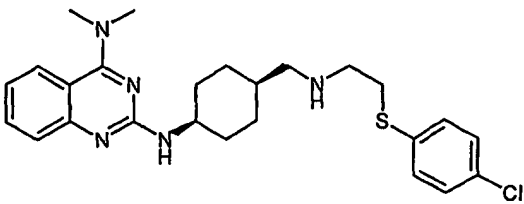
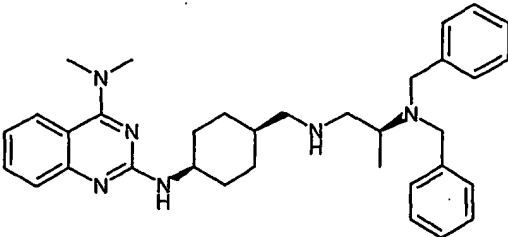
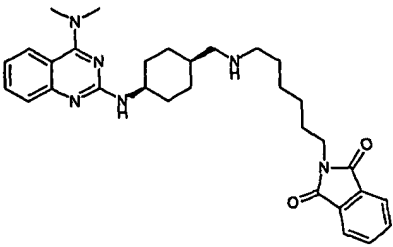
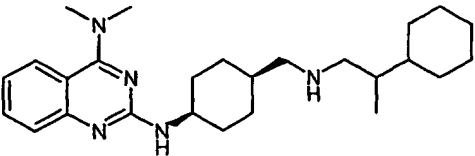
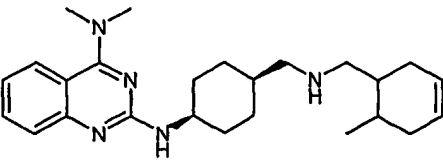
Example No.	Structure	APCI-MS
2297		422 (M + H)
2298		474 (M + H)
2299		476 (M + H)
2300		516 (M + H)
2301		448 (M + H)

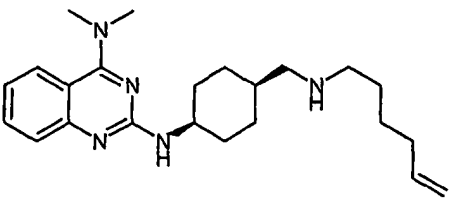
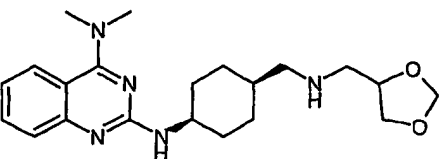
Example No.	Structure	APCI-MS
2302		470 (M + H)
2303		446 (M + H)
2304		488 (M + H)
2305		460 (M + H)
2306		434 (M + H)

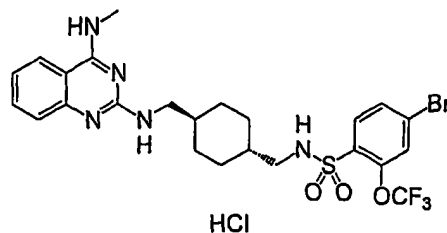
Example No.	Structure	APCI-MS
2307		582 (M + H)
2308		442 (M + H)
2309		419 (M + H)
2310		434 (M + H)
2311		482 (M + H)

Example No.	Structure	APCI-MS
2312		418 (M + H)
2313		446 (M + H)
2314		482 (M + H)
2315		472 (M + H)
2316		437 (M + H)

Example No.	Structure	APCI-MS
2317		434 (M + H)
2318		418 (M + H)
2319		462 (M + H)
2320		460 (M + H)
2321		554 (M + H)

Example No.	Structure	APCI-MS
2322		470 (M + H)
2323		537 (M + H)
2324		529 (M + H)
2325		424 (M + H)
2326		408 (M + H)

Example No.	Structure	APCI-MS
2327	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCCC=C</chem>	382 (M + H)
2328	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4OCCO4</chem>	386 (M + H)

Example 2329

***trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride**

Step A: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid.

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (3.14 g, 20 mmol) in THF (20 mL) and 1 M aqueous sodium hydroxide (42 mL) was added a solution of 4-bromo-2-trifluoromethoxy benzenesulfonyl chloride (6.9 g, 20.4 mmol) in THF (20 mL) and the mixture was stirred for 2 hr at ambient temperature. The resulting mixture was concentrated and 1 M aqueous HCl (45 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.18 g, 78%) as a white powder.

ESI MS *m/e* 460/462 *M* + *H*⁺ ; ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.00 (brs, 1 H), 7.99 (brs, 1 H), 7.84-7.80 (m, 3 H), 2.72 (d, *J* = 6.3 Hz, 2 H), 2.10 (m, 1 H), 1.86 (m, 2 H), 1.71 (m, 2 H), 1.31 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

Step B: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide.

A solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.14 g, 15.5 mmol) and triethylamine (2.35 mL, 16.9 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (1.62 mL, 17 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, aqueous ammonia (27 mL) was added dropwise and the mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated under reduced pressure and the concentrate was treated with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-

benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide as a white solid (4.2 g, 59%).

ESI MS m/e 459/461 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.98 (brs, 1 H), 7.84-7.80 (m, 3 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 2.72 (d, $J = 6.5$ Hz, 2 H), 1.98 (m, 1 H), 1.70 (m, 4 H), 1.29 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.

To a solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide (4.2 g, 9.2 mmol) in THF (40 mL) was added a solution of 1 M BH_3 in THF (32 mL, 32 mmol) over 40 min. The mixture was refluxed for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the resulting mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (28 mL) and the mixture was concentrated. To the residue was added MeOH (28 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et_2O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH_2Cl_2 (twice), the organic layers combined, dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide as a white solid (3.0 g, 74%).

ESI MS m/e 445/447 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.84-7.79 (m, 3 H), 3.42 (brs, 2 H), 2.72 (d, $J = 6.8$ Hz, 2 H), 2.33 (d, $J = 6.5$ Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.09 (m, 1 H), 0.80 (m, 4 H).

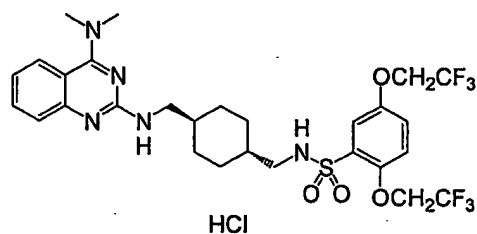
Step D: Synthesis of *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride.

A mixture of (2-chloro-quinazolin-4-yl)-methylamine obtained in step A of example 50 (58 mg, 0.3 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide amide (133 mg, 0.3 mmol) in 2-propanol (0.5 mL) was stirred at reflux for 24 hr. The mixture was cooled and the resulting white solid was collected by filtration and washed with 2-propanol to give *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride as a white solid (121 mg, 67%).

ESI MS m/e 602/604 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 12.61 (brs, 1 H), 9.70

(brs, 1 H), 8.26 (d, $J = 8.1$ Hz, 1 H), 8.15 (brs, 1 H), 8.02 (t, $J = 5.7$ Hz, 1 H), 7.84-7.74 (m, 4 H), 7.41 (m, 1 H), 3.32 (m, 2 H), 3.07 (d, $J = 3.5$ Hz, 3 H), 2.73 (t, $J = 6.2$ Hz, 2 H), 1.77 (m, 4 H), 1.53 (m, 1 H), 1.32 (m, 1 H), 0.96 (m, 2 H), 0.82 (m, 2 H).

Example 2330



***trans*-N-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride**

Step A: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid.

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (1.5 g, 10 mmol) in THF (10 mL) and 1 M aqueous sodium hydroxide (27 mL) was added a solution of 2,5-bis(2,2,2-trifluoroethoxy) benzenesulfonyl chloride (3.8 g, 10.25 mmol) in THF (10 mL) dropwise and the mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated and 1 M aqueous HCl (22.5 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid as a white powder (2.8 g, 57%).

ESI MS m/e 494 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36 (m, 3 H), 7.23 (brs, 1 H), 4.88 (m, 4 H), 2.73 (m, 2 H), 2.10 (m, 1 H), 1.87 (m, 2 H), 1.72 (m, 2 H), 1.30 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

Step B: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide.

A solution of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid (2.78 g, 5.63 mmol) and triethylamine (1.9 mL,

13.6 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (0.586 mL, 6.2 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, 25% aqueous ammonia (10 mL) was added dropwise. The mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated under reduced pressure and the concentrate was diluted with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide as a white solid (2.7 g, 98%).

ESI MS m/e 493 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36 (m, 3 H), 7.23 (t, $J = 6.1$ Hz, 1 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 4.88 (m, 4 H), 2.74 (t, $J = 6.4$ Hz, 2 H), 1.99 (m, 1 H), 1.75 (m, 4 H), 1.28 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide.

To a solution of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide (2.7 g, 5.5 mmol) in THF (20 mL) was added a solution of 1 M BH_3 in THF (20 mL, 20 mmol) over 40 min. The mixture was stirred at reflux for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (50 mL) and the mixture was concentrated. To the residue was added MeOH (50 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et_2O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH_2Cl_2 (twice), the combined organic layers were dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide as a white solid (1.5 g, 57%).

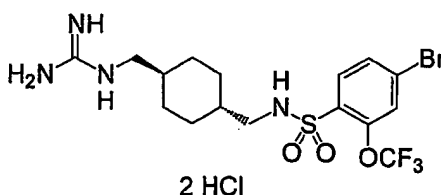
ESI MS m/e 479 $M + H^+$; 1H NMR (500 MHz, DMSO- d_6) δ 7.36-7.32 (m, 3 H), 6.62 (brs, 1 H), 4.88-4.78 (m, 4 H), 3.42 (b, 2 H), 2.73 (d, $J = 6.6$ Hz, 2 H), 2.34 (d, $J = 6.3$ Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.10 (m, 1 H), 0.77 (m, 4 H).

Step D: Synthesis of *trans*-*N*-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride.

A mixture of (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (41.4 mg, 0.2 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide (95.6 mg, 0.2 mmol) in 2-propanol was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was purified by column chromatography (silica gel) to give the product as a white foam. The product was dissolved in CH₂Cl₂ and treated with 1 M HCl in Et₂O. The mixture was concentrated to give *trans*-*N*-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride as a white foam (101 mg, 78%).

ESI MS *m/e* 650 M + H⁺; ¹H NMR (500 MHz, DMSO-d₆) δ 8.16 (d, *J* = 8.2 Hz, 1 H), 8.00 (brs, 1 H), 7.78 (t, *J* = 7.9, 1 H), 7.44 (brs, 1 H), 7.34 (m, 4 H), 7.24 (t, *J* = 5.9 Hz, 1 H), 4.88 (m, 4 H), 3.32 (s, 6 H), 3.29 (m, 2 H), 2.75 (t, *J* = 6.2 Hz, 2 H), 1.74 (m, 4 H), 1.52 (m, 1 H), 1.32 (m, 1 H), 0.94 (m, 2 H), 0.83 (m, 2 H).

Example 2331



***trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride**

Step A: Synthesis of *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester.

To a solution of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide obtained in step C of example 2329 (45 mg, 0.1 mmol) and triethylamine (14 μL, 0.1 mmol) in CH₂Cl₂ (5 mL) was added (*tert*-butoxycarbonylamino-trifluoromethanesulfonylimino-methyl)-carbamic acid *tert*-butyl ester (39.1 mg, 0.1 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was purified by column chromatography (silica gel,

CH₂Cl₂ to 10% MeOH in CH₂Cl₂) to give *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-

cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid

tert-butyl ester as a white solid (63 mg, 92%).

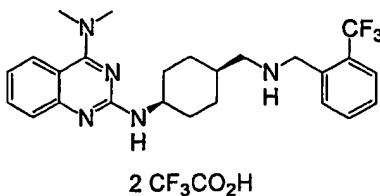
ESI MS *m/e* 687/689 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.45 (s, 1 H), 8.22 (t, *J* = 5.6 Hz, 1 H), 7.97 (t, *J* = 5.6 Hz, 1 H), 7.99-7.79 (m, 3 H), 3.13 (t, *J* = 6.4 Hz, 2 H), 2.72 (t, *J* = 6 Hz, 2 H), 1.70 (m, 4 H), 1.46 (s, 9 H), 1.38 (s, 9 H), 1.31 (m, 2 H), 0.83 (m, 4 H).

Step B: Synthesis of *trans*-4-bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride.

A solution of *trans*-[({4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester (53 mg, 0.077 mmol) in 50% TFA in CH₂Cl₂ (2 mL) was stirred at ambient temperature for 3 hr and the reaction mixture was concentrated. To the residue was added a solution of 1 M HCl in Et₂O (0.5 mL) and the mixture was concentrated to give *trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride as a white solid (29 mg, 68%).

ESI MS *m/e* 487/489 *M* + *H*⁺; ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.01 (t, *J* = 5.5 Hz, 1 H), 7.84 (m, 3 H), 7.68 (m, 1 H), 7.30 (m, 2 H), 6.85 (m, 2 H), 2.94 (t, *J* = 6.1 Hz, 2 H), 2.74 (t, *J* = 6.1 Hz, 2 H), 1.71 (m, 2 H), 1.31 (m, 4 H), 0.86 (m, 4 H).

Example 2332



cis-*N*^{*r*},*N*^{*r*}-Dimethyl-*N*^{*r*}-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid.

To a solution of *cis*-4-amino-cyclohexanecarboxylic acid (50 g, 350 mmol) in THF

(200 mL) and 1 M aqueous sodium hydroxide (380 mL, 380 mmol) was added (Boc)₂O (83.5 g, 360 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was cooled to 0 °C followed by acidification with 1 M HCl (pH = 3). The resulting white solid was filtered, washed with water and hexanes to give *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (71 g, 83%) as a white solid. ESI MS *m/e* 244 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.00 (brs, 1 H), 6.74 (d, *J* = 4.25, 1 H), 3.30 (brs, 1 H), 2.35 (m, 1 H), 1.87 (m, 2 H), 1.55-1.37 (m, 15 H).

Step B: Synthesis of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester.

To a solution cooled at 0°C of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (68.0 g, 280 mmol) and triethylamine (31.1 g, 307 mmol) in THF (300 mL) was added ethyl chloroformate (29.3 mL, 308 mmol) dropwise. After stirring at 0 °C for 30 min, 25% aqueous ammonia (168 mL) was added dropwise. The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was extracted with EtOAc (three times). The combined organic layer was washed with saturated aqueous NaHCO₃, 1 M HCl, brine, and water, dried over Na₂SO₄, filtered, and concentrated to give *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62.0 g, 88%) as a white solid.

ESI MS *m/e* 243 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.10 (brs, 1 H), 6.69 (b, 2 H), 3.41 (brs, 1 H), 2.14 (m, 1 H), 1.79 (m, 2 H), 1.59 (m, 2 H), 1.45-1.37 (m, 13 H).

Step C: Synthesis of *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride.

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62 g, 256 mmol) in CH₂Cl₂ (250 mL) was added TFA (250 mL) and the mixture was stirred at ambient temperature for 1 hr. The mixture was concentrated and 2 M HCl in Et₂O (150 mL) was added to give a white precipitate. The mixture was concentrated to give *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (45 g, 98%) as a white solid.

ESI MS *m/e* 143 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.08 (m, 3 H), 7.28 (s, 1 H), 6.78 (s, 1 H), 3.10 (m, 1 H), 2.24 (m, 1 H), 1.90 (m, 2 H), 1.66 (m, 4 H), 1.50 (m, 2 H).

Step D: Synthesis of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide.

A solution of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of

example 1 (31.05 g, 150 mmol) and *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (26.7 g, 150 mmol) in pyridine (150 mL) was stirred at reflux for overnight. The reaction mixture was concentrated and residue was dissolve in CH₂Cl₂. The organic layer was washed with saturated aqueous NaHCO₃ and the aqueous layer was extracted with CH₂Cl₂. The organic layer was dried over Na₂SO₄, filtered and concentrated. The residue was purified by column chromatography (silica gel, 2% to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give a slightly brown solid and the solid was recrystallized from CH₂Cl₂ to give *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (20.6 g, 44%) as yellow crystals.

ESI MS *m/e* 314 M + H⁺ ; ¹H NMR (400 MHz, DMSO-d₆) δ 8.19 (brs, 1 H), 8.15 (d, *J* = 8.4 Hz, 1 H), 7.77 (t, *J* = 8.0 Hz, 1 H), 7.42 (d, *J* = 7.2 Hz, 1 H), 7.35 (t, *J* = 8.4 Hz, 1 H), 7.21 (s, 1 H), 6.74 (s, 1 H), 4.12 (m, 1 H), 3.46 (m, 6 H), 2.24 (m, 1 H), 1.79-1.61 (m, 8 H).

Step E: Synthesis of *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine.

To a solution of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (18.78 g, 60 mmol) in THF (200 mL) was added a solution of 1 M BH₃ in THF (300 mL, 300 mmol). The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to 0 °C, 4 M HCl in EtOAc (100 mL) and MeOH (200 mL) were added. The mixture was concentrated. The mixture was treated with 1 M aqueous sodium hydroxide and the aqueous layer was extracted with CH₂Cl₂. The organic layer was dried over sodium sulfate, concentrated, and purified by column chromatography (silica gel, 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine as a white solid (10.6 g, 59%).

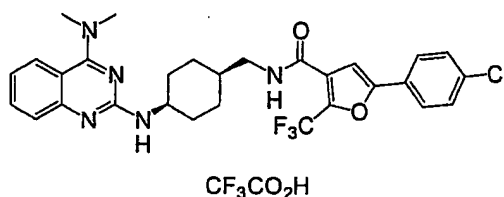
ESI MS *m/e* 300 M + H⁺ ; ¹H NMR (400 MHz, DMSO-d₆) δ 7.84 (d, *J* = 8.4 Hz, 1 H), 7.46 (t, *J* = 6.8 Hz, 1 H), 7.26 (d, *J* = 8.4 Hz, 1 H), 6.99 (t, *J* = 6.8 Hz, 1 H), 6.28 (brs, 1 H), 4.02 (m, 1 H), 3.19 (m, 6 H), 2.47 (d, *J* = 6.8 Hz, 2 H), 2.73 (m 2 H), 1.68-1.33 (m, 9 H).

Step F: Synthesis of *cis*-N⁴,N⁴-dimethyl-N²-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine (33 mg, 0.11 mmol) and 2-trifluoromethyl benzaldehyde (17.41 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature for 3 hr. To the mixture was added NaBH(OAc)₃ (85 mg, 0.4 mmol) and the mixture was stirred at ambient temperature for overnight. This resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-*N*⁴,*N*⁴-dimethyl-*N*²-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid (41.4 mg, 60%) as a white solid.

ESI MS *m/e* 458 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 13.12 (brs, 1 H), 8.94 (b, 2 H), 8.65 (d, *J* = 6.8 Hz, 1 H), 8.16 (d, *J* = 8.8 Hz, 1 H), 7.77-7.66 (m, 5 H), 7.41 (d, *J* = 8.4 Hz, 1 H), 7.35 (t, *J* = 8 Hz, 1 H), 4.22 (s, 2 H), 4.17 (m, 1 H), 3.46 (b, 6 H), 2.94 (m, 2 H), 1.87-1.44 (m, 9 H).

Example 2333



***cis*-5-(4-Chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid**

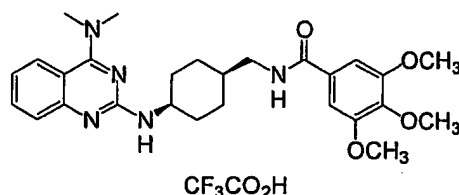
Step A: Synthesis of *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid.

A solution of *cis*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (30 mg, 0.1 mmol), 5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-acid chloride (37 mg, 0.12 mmol), and pyridine (12 μL, 0.15 mmol) in DMF (0.5 mL) was stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.8 mL) and the mixture was purified by preparative

HPLC. The pure fractions were combined and lyophilized to give *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid (17.5 mg, 26%) as a white solid.

ESI MS m/e 572 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.30 (brs, 1 H), 8.65 (t, J = 6.8 Hz, 1 H), 8.19 (brs, 1 H), 8.14 (d, J = 8.0 Hz, 1 H), 7.83-7.30 (m, 8 H), 4.1 (m, 1 H), 3.46 (b, 6 H), 3.09 (m, 2 H), 1.77-1.38 (m, 9 H).

Example 2334



***cis*-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid**

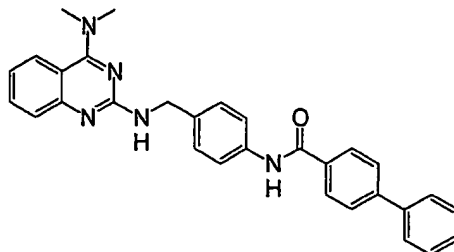
Step A: Synthesis of *cis*-N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid.

To HOBt-6-carboxamidomethyl polystyrene 200-400 mesh (77 mg, 0.1 mmol) were added a solution of 0.3 M PyBroP in DMF (1 mL, 0.3 mmol), 3,4,5-trimethoxybenzoic acid (63 mg, 0.3 mmol), and diisopropylethylamine (85 μ L, 0.5 mmol). The mixture was stirred at ambient temperature for 5 hr. The resin was washed with DMF (3 times), CH_2Cl_2 (3 times), MeOH (3 times), CH_2Cl_2 (2 times), and DMF (2 times). To the resin was added *cis*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (28 mg, 0.09 mmol) in DMF (0.5 mL) and the mixture was stirred at ambient temperature for overnight. The resin was filtered and washed with 0.5 mL DMSO (2 times). The combined filtrates were purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis* N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid (7.4 mg, 12%) as a white solid.

ESI MS m/e 494 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.25 (brs, 1 H), 8.45 (t, J = 5.6 Hz, 1 H), 8.17 (brs, 1 H), 8.14 (d, J = 8.0 Hz, 1 H), 7.76 (t, J = 8.4 Hz, 1 H), 7.42 (d, J

= 7.2 Hz, 1 H), 7.34 (t, J = 7.6 Hz, 1 H), 7.15 (s, 2 H), 4.13 (m, 1 H), 3.44 (s, 3 H), 3.39 (s, 3 H), 3.20 (m, 2 H), 1.77-1.37 (m, 9 H).

Example 2335



Biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide

Step A: Synthesis of (4-amino-benzyl)-carbamic acid *tert*-butyl ester.

A solution of 4-aminomethyl-phenylamine (12.2 g, 100 mmol) and (Boc)₂O (21.8 g, 100 mmol) in CH₂Cl₂ (100 mL) was stirred at ambient temperature for overnight. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% MeOH in CH₂Cl₂) to give (4-amino-benzyl)-carbamic acid *tert*-butyl ester (11.6 g, 52%) as a slightly yellow solid.

ESI MS m/e 223 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.27 (t, J = 6.0 Hz, 1 H), 6.86 (d, J = 8.0 Hz, 2 H), 6.47 (d, J = 6.4 Hz, 2 H), 4.89 (s, 2 H), 3.91 (d, J = 6.0 Hz, 2 H), 1.39 (s, 9 H).

Step B: Synthesis of biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride.

To a solution of (4-amino-benzyl)-carbamic acid *tert*-butyl ester (1.11 g, 5 mmol), biphenyl carboxylic acid (0.99 g, 5 mmol), EDC (1.2 g, 6.25 mmol), and HOAt (0.82 g, 6 mmol) in CH₂Cl₂ (10 mL) was added triethylamine (pH = 10) and the mixture was stirred at ambient temperature for overnight. The organic layer was washed with saturated aqueous NaHCO₃, 1 M aqueous HCl, water, dried over Na₂SO₄, filtered, and concentrated. The residue was dissolved in 50% TFA in CH₂Cl₂ (10 mL) and the mixture was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and diluted with 1 M HCl in Et₂O (5 mL). The mixture was concentrated to give biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (828 mg, 49%).

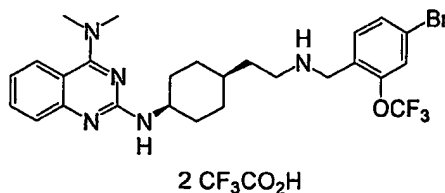
ESI MS m/e 303 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.40 (s, 1 H), 8.34 (b, 3 H), 8.07 (d, $J = 8.0$ Hz, 2 H), 7.83-7.73 (m, 6 H), 7.51-7.38 (m, 5 H), 4.0 (q, $J = 5.6$ Hz, 2 H).

Step C: Synthesis of biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (42 mg, 0.2 mmol) and biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (49 mg, 0.14 mmol) in 2-propanol (1 mL) and triethylamine (200 μ L) was stirred at reflux for 2 days. The resulting mixture was concentrated and purified by column chromatography (silica gel, CH_2Cl_2 to 10% 2 M $NH_3/MeOH$ in CH_2Cl_2) to give biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide (10 mg, 15%) as a white solid.

ESI MS m/e 474 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.19 (s, 1 H), 8.02 (d, $J = 7.2$ Hz, 2 H), 7.86 (d, $J = 8.4$ Hz, 1 H), 7.80 (d, $J = 8.4$ Hz, 2 H), 7.73 (d, $J = 7.2$ Hz, 2 H), 7.68 (d, $J = 7.6$ Hz, 2 H), 7.50-7.15 (m, 8 H), 7.01 (t, $J = 8.4$ Hz, 1 H), 4.51 (d, $J = 6.4$ Hz, 2 H), 3.30 (s, 3 H), 3.2 (s, 3 H).

Example 2336



***cis*-N²-{4-[2-(4-Bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester.

To a solution of *cis*-[4-(2-amino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (4.84 g, 20 mmol) in CH_2Cl_2 (50 mL) and triethylamine (3.06 mL, 22 mmol) was added benzyl chloroformate (3.13 mL, 22 mmol) and the mixture was stirred for 4 hr. The resulting mixture was washed with water, 1 M aqueous HCl, dried over Na_2SO_4 , filtered and concentrated. The residue was purified by column chromatography (silica gel,

CH₂Cl₂ to 10% MeOH in CH₂Cl₂) to give *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.46 g, 73%) as a colorless oil.

ESI MS *m/e* 377 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.36-7.24 (m, 5 H), 7.19 (t, *J* = 5.6 Hz, 1 H), 6.76 (d, *J* = 6.8 Hz, 1 H), 4.91 (s, 2 H), 3.40 (m, 1 H), 2.99 (m, 2 H), 1.44-1.33 (m, 20H).

Step B: Synthesis of *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester.

A solution of *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.26 g, 14 mmol) in 50% TFA in CH₂Cl₂ (60 mL) was stirred at ambient temperature for 1 hr. The mixture was concentrated and the residue was diluted with saturated aqueous NaHCO₃. The aqueous layer was extracted with CH₂Cl₂ (three times). The organic layer was dried over Na₂SO₄ and concentrated to give *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.5 g, 91%) as a colorless oil.

ESI MS *m/e* 277 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.72 (b, 2 H), 7.34-7.27 (m, 5 H), 7.21 (t, *J* = 5.2 Hz, 1 H), 4.97 (s, 2 H), 3.14 (m, 1 H), 2.99 (q, *J* = 6.4 Hz, 2 H), 1.58-1.34 (m, 11 H).

Step C: Synthesis of *cis*{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-carbamic acid benzyl ester.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (2.45 g, 10.2 mmol) and *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.3 g, 10.2 mmol) and triethylamine (1.65 mL, 10.2 mmol) in 2-propanol (15 mL) was heated at 170 °C for 45 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-carbamic acid benzyl ester (4.48g, 85%) as a yellow oil.

ESI MS *m/e* 448 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 8.07-7.20 (m, 11 H), 4.98 (s, 2 H), 4.08 (m, 1 H), 3.39 (b, 6 H), 3.04 (m, 2 H), 1.7-1.3 (m, 11 H).

Step D: Synthesis of *cis*-N²-[4-(2-amino-ethyl)-cyclohexyl]-N²,N²-dimethyl-quinazoline-2,4-diamine.

To a solution of *cis*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-

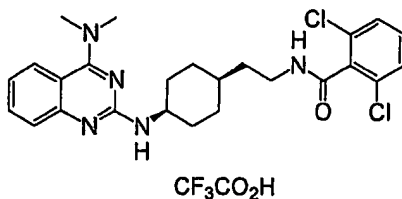
ethyl}-carbamic acid benzyl ester (4.47 g, 10 mmol) in EtOH (20 mL) was added 1,4-cyclohexadiene (20 mL) and 200 mg of 10% Pd/C. The reaction mixture was stirred at ambient temperature for 18 hr, filtered through pad of celite, and concentrated. The residue was purified by column chromatography (silica gel, 5% to 15% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-N²-[4-(2-amino-ethyl)-cyclohexyl]-N',N'-dimethyl-quinazoline-2,4-diamine (2.41g, 77%) as a yellow oil.

ESI MS m/e 314 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 7.82 (d, *J* = 8.0 Hz, 1 H), 7.44 (t, *J* = 6.8 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 6.97 (t, *J* = 6.8 Hz, 1 H), 6.31 (brs, 1 H), 3.97 (m, 1 H), 3.37 (b, 2 H), 3.17 (s, 3), 3.14 (s, 3 H), 2.62 (t, *J* = 7.6 Hz, 2 H), 1.68-1.31 (m, 11 H).

Step E: Synthesis of *cis*-N²-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N',N'-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*-N²-[4-(2-amino-ethyl)-cyclohexyl]-N',N'-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 4-bromo-2-trifluoromethoxy benzaldehyde (26.9 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, NaBH(OAc)₃ (85 mg, 0.4 mmol) was added and the resulting mixture was stirred at ambient temperature for overnight. The reaction mixture was quenched with 50% DMSO in water (2 mL). The mixture was concentrated and purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-N²-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N',N'-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (32.2 mg, 41%) as a white solid.

ESI MS m/e 566/568 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 12.76 (brs, 1 H), 8.81 (b, 2 H), 8.43 (m, 1 H), 8.09 (d, *J* = 8.4 Hz, 1 H), 7.71-7.56 (m, 4 H), 7.35 (d, *J* = 8.0 Hz, 1 H), 7.29 (t, *J* = 8.0 Hz, 1 H), 4.15 (m, 3 H), 3.39 (m, 6 H), 2.97 (m, 2 H), 1.67-1.30 (m, 11 H).

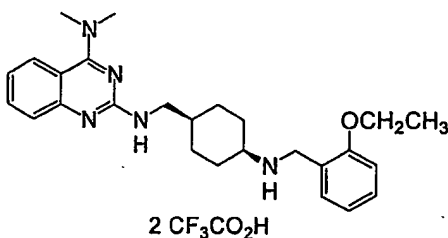
Example 2337

***cis*-2,6-Dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid**

Step A: Synthesis of *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid.

To a solution of *cis*-*N*²-[4-(2-amino-ethyl)-cyclohexyl]-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 2,6-dichlorobenzoyl chloride (20.7 mg, 0.1 mmol) in DMF (0.5 mL) was added triethylamine (20 uL, 0.14 mmol). After stirring the mixture at ambient temperature for 6 hr, DMSO (0.5 mL) was added and the mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid (17.6 mg, 29%) as a white solid.

ESI MS *m/e* 486 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.93 (brs, 1 H), 8.26 (t, *J* = 5.2 Hz, 1 H), 8.14 (d, *J* = 8.0 Hz, 1 H), 7.95 (brs, 1 H), 7.76 (t, *J* = 8.4 Hz, 1 H), 7.52-7.31 (m, 5 H), 4.15 (m, 1 H), 3.45 (b, 6 H), 3.29 (m, 2 H), 1.76-1.31 (m, 11 H).

Example 2338

***cis*-*N*²-[4-(2-Ethoxy-benzylamino)-cyclohexylmethyl]-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid tert-butyl ester.

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester obtained in step B of example 2332 (9.68 g, 40 mmol) in THF (100 mL) was added a solution of 1 M BH₃ in THF (80 mL, 80 mmol) over 30 min. The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to ambient temperature, 1 M aqueous sodium hydroxide was carefully added. The solvents were removed under reduced pressure and the aqueous layer was extracted with CH₂Cl₂ (twice). The organic layer was dried over sodium sulfate and concentrated under reduced pressure to give *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester as colorless oil (5.16 g, 57%).

ESI MS *m/e* 229 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 6.67 (d, *J* = 6.8 Hz, 1 H), 3.43 (m, 1 H), 2.41 (d, *J* = 6.4 Hz, 2 H) 1.49-1.22 (m, 18 H).

Step B: Synthesis of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester.

A mixture of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester (1.14 g, 5 mmol), (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (1.035 g, 5 mmol), and triethylamine (1.5 mL, 11 mmol) in 2-propanol (2.5 mL) was heated at 170 °C for 35 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH₂Cl₂ to 10% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.28 g, 80%) as a white solid.

ESI MS *m/e* 400 M + H⁺; ¹H NMR (400 MHz, DMSO-d₆) δ 8.04-7.06 (m, 4 H), 6.77 (d, *J* = 6.0 Hz, 1 H), 3.40-3.16 (m, 9 H), 1.70-1.37 (m, 18 H).

Step C: Synthesis of *cis*-N²-(4-amino-cyclohexylmethyl)-N¹,N¹-dimethyl-quinazoline-2,4-diamine.

A solution of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.2 g, 3 mmol) in 50% TFA in CH₂Cl₂ (20 mL) was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and the residue was diluted with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH₂Cl₂ (twice). The combined organic layer was dried over Na₂SO₄, filtered and concentrated to give *cis*-N²-(4-amino-cyclohexylmethyl)-N¹,N¹-dimethyl-quinazoline-2,4-diamine (0.88 g, 98%) as a white solid.

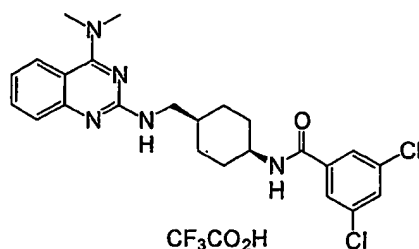
ESI MS m/e 300 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.85 (d, $J = 7.6$ Hz, 1 H), 7.47 (t, $J = 6.8$ Hz, 1 H), 7.27 (brs, 1 H), 7.0 (t, $J = 7.2$ Hz, 1 H), 6.66 (brs, 1 H), 3.33-3.14 (m, 9 H), 1.69-1.48 (m, 9 H).

Step D: Synthesis of *cis*- N^2 -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A solution of *cis*- N^2 -(4-amino-cyclohexylmethyl)- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine (30 mg, 0.1 mmol) and 2-ethoxy benzaldehyde (15 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, NaBH(OAc)₃ (85 mg, 0.4 mmol) was added and the mixture was stirred at ambient temperature for overnight. The resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*- N^2 -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- N^4 , N^4 -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (33 mg, 50%) as a white solid.

ESI MS m/e 434 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 13.03 (brs, 1 H), 8.79 (brs, 1 H), 8.49 (m, 2 H), 8.15 (d, $J = 8.4$ Hz, 1 H), 7.77 (t, $J = 7.6$ Hz, 1 H), 7.40-7.33 (m, 4 H), 7.07 (d, $J = 7.6$ Hz, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 4.11-4.06 (m, 4 H), 3.47-3.41 (m, 8 H), 3.15 (m, 1 H), 1.90-1.60 (m, 9 H), 1.37 (t, $J = 7.2$ Hz, 3 H).

Example 2339



***cis*-3,5-Dichloro- N -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid**

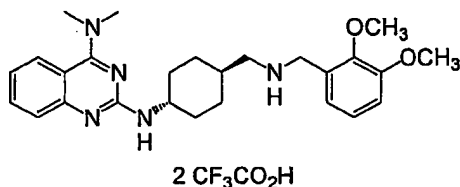
Step A: Synthesis of *cis*-3,5-dichloro- N -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid.

A solution of *cis*- N^2 -(4-amino-cyclohexylmethyl)- N^4 , N^4 -dimethyl-quinazoline-2,4-

diamine (30 mg, 0.1 mmol) and 3,5-dichlorobenzoylchloride (20.9 mg, 0.1 mmol) and pyridine (12 μ L, 0.25 mmol) in DMSO (1 mL) was stirred at ambient temperature for overnight. The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-3,5-dichloro-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid. (18 mg, 31%) as a white solid.

ESI MS m/e 472 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.13 (brs, 1 H), 8.34 (d, $J = 7.2$ Hz, 1 H), 8.15 (d, $J = 8.8$ Hz, 1 H), 8.06 (brs, 1 H), 7.82-7.73 (m, 4 H), 7.45 (d, $J = 7.6$ Hz, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 3.9 (m, 1 H), 3.47-3.25 (m, 8 H), 1.83-1.56 (m, 9 H).

Example 2340



***trans*-*N*²-{4-[(2,3-Dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid.

To a solution of *trans*-4-amino-cyclohexanecarboxylic acid (37.7 g, 0.24 mol) in a mixture of dioxane (250 ml) and water (200 ml) cooled in an ice bath were added 1 M aqueous sodium hydroxide (10.07 g, 0.25 mol) and (Boc)₂O (57.6 g, 0.26 mol). The reaction mixture was stirred at ambient temperature. After 3 hr, the mixture was concentrated and the residue was dissolved in water. The aqueous layer was washed with Et₂O (3 times). The aqueous layer was cooled in an ice bath and acidified with 1 M aqueous HCl (pH = 2) and the resulting white precipitate was dried to give *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (47.4 g, 76.8%) as a white solid.

ESI MS m/e 258 $M + H^+$; 1H NMR (400 MHz, CDCl₃) δ 11.95 (brs, 1 H), 6.79 (t, $J = 6.0$ Hz, 1 H), 2.76 (t, $J = 6.0$ Hz, 2 H), 2.11 (m, 1 H), 1.87 (m, 2 H), 1.69 (m, 2 H), 1.36 (s,

9 H), 1.27 (m, 3 H), 0.9 (m, 2 H).

Step B: Synthesis of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester.

To a solution of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (46.9 g, 0.18 mol) in benzene (300 mL) were added triethylamine (24.2 g, 0.24 mol) and diphenylphosphoryl azide (55.9 g, 0.20 mol). The reaction mixture was stirred at 80 °C for 1 hr. To the mixture was added benzyl alcohol (25.9 g, 0.24 mol) and stirred at 100 °C for 4 hr. The mixture was subsequently cooled to ambient temperature for overnight, concentrated, and the resulting pale orange solid dissolved in EtOAc. The organic layer was washed with water (three times), concentrated, and the residue was purified by column chromatography (silica gel, 50% EtOAc in hexane) to give *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (66.7g, 100%) as a white solid.

ESI MS m/e 363 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 7.24-7.23 (m, 5 H), 5.06 (s, 2 H), 4.57 (m, 2 H), 3.44 (brs, 1 H), 2.97 (t, J = 6.4 Hz, 2 H), 2.04 (m, 2 H), 1.79 (m, 2 H), 1.43 (s, 9 H), 1.08-0.76 (m, 5 H).

Step C: Synthesis of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester.

To a solution of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (5.32 g, 0.015 mol) in EtOH (200 mL) was added 10% Pd/C (50 mg). The mixture was stirred at ambient temperature under hydrogen atmosphere for 4 hr. The resulting mixture was filtered through a pad of celite and concentrated. The residue was purified by column chromatography (silica gel, 3% 2 M NH₃/MeOH in CH₂Cl₂) to give *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester as a colorless solid (3.197 g, 95.4%).

ESI MS m/e 229 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 8.44 (brs, 1 H), 4.59 (b, 1 H), 2.96 (m, 2 H), 2.08 (m, 2 H), 1.83 (m, 2 H), 1.43 (s, 9 H), 1.08 (m, 5 H).

Step D: Synthesis of *trans*-N²-(4-aminomethyl-cyclohexyl)-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

A mixture of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester

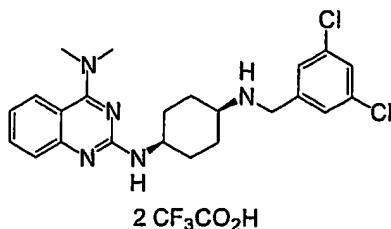
(0.24 g, 1 mmol) and (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.32 g, 1.4 mmol) in 2-propanol (5 mL) was heated to 170 °C for 30 min using a Smith Microwave Synthesizer. This procedure was repeated 19 times. The reaction mixtures were combined and purified by column chromatography (silica gel) to give 1.13 g of a yellow solid. The yellow solid was dissolved in 50% TFA in CH₂Cl₂ (20 mL) and the mixture was stirred at ambient temperature. After 10 hours, the mixture was concentrated and the residue was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (0.49 g, 5%) as a white solid.

ESI MS *m/e* 300 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.16 (d, *J* = 5.6 Hz, 1 H), 8.11 (m, 2 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.51 (t, *J* = 7.6 Hz, 1 H), 7.41 (d, *J* = 8.0 Hz, 1 H), 7.18 (t, *J* = 6.8 Hz, 1 H), 3.8 (brs, 1 H), 3.47 (s, 6 H), 2.10 (m, 2 H), 1.92 (m, 2 H), 1.42-1.12 (m, 5 H).

Step E: Synthesis of *trans*-*N*²-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

A mixture of 2,3-dimethoxy benzaldehyde (15 mg, 0.09 mmol), *trans*-*N*²-(4-aminomethyl-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (28 mg, 0.053 mmol), NaBH(OAc)₃ (76 mg, 0.36 mmol), and MeOH (2 mL) was heated at 100 °C for 40 seconds using a Smith Microwave Synthesizer. The resulting mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*²-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (10.2 mg, 28 %).

ESI MS *m/e* 450 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.68 (d, *J* = 6.0 Hz, 1 H), 9.41 (brs, 1 H), 7.85 (d, *J* = 7.6 Hz, 1 H), 7.52 (t, *J* = 7.2 Hz, 1 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.19 (t, *J* = 7.2 Hz, 1 H), 7.09 (t, *J* = 8.0 Hz, 1 H), 6.98 (d, *J* = 7.2 Hz, 1 H), 6.90 (d, *J* = 7.6 Hz, 1 H), 4.16 (s, 2 H), 3.96 (s, 3 H), 3.87 (s, 3 H), 3.75 (m, 1 H), 3.47 (m, 6 H), 2.80 (m, 2 H), 2.11 (m, 2 H), 1.86 (m, 2 H), 1.48-1.50 (m, 5 H).

Example 2341

***cis*-N²-[4-(3,5-Dichloro-benzylamino)-cyclohexyl]-N⁴,N⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester.

To a suspension of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (50.0 g, 206 mmol) in benzene were added triethylamine (26.9 g, 266 mmol) and phosphorazidic acid diphenyl ester (62.2 g, 226 mmol). The reaction mixture was stirred at 80°C for 1 hr. Benzyl alcohol (31.4 g, 290 mmol) was added and the mixture was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was dissolved in EtOAc and H₂O. The organic layer was separated and the aqueous layer was extracted with EtOAc (twice). The combined organic layer was dried over MgSO₄, filtered, concentrated, and purified by flash chromatography (silica gel, 30% EtOAc in hexane) to give *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester (54.1 g, 76%) as a colorless oil.

ESI MS *m/e* 349 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.34-7.28 (m, 5 H), 7.12 (d, *J* = 5.6 Hz, 1 H), 6.62 (brs, 1 H), 4.98 (s, 2 H), 3.39-3.37 (m, 2 H), 1.60-1.45 (m, 8 H), 1.37 (s, 9 H).

Step B: Synthesis of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.

Using the procedure for the step C of example 2340, the title compound was obtained.

ESI MS *m/e* 215 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 6.60 (d, *J* = 6.0 Hz, 1 H), 3.30-3.28 (m, 1 H), 2.74 (s, 1 H), 1.59-1.51 (m, 2 H), 1.45-1.37 (m, 15 H).

Step C: Synthesis of *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-

carbamic acid *tert*-butyl ester.

A solution of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.3 mmol), (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B in example 1 (0.53, 2.6 mmol), diisopropylethylamine (1.22 mL, 7.0 mmol) and 2-propanol (1.0 mL) was heated using a Smith Microwave Synthesizer at 170 °C for 1 hour. This reaction procedure was repeated 39 more times and the resulting reaction mixtures were combined. The mixture was concentrated and the residue was purified by column chromatography (silica gel, 2% to 4% 2 M NH₃/MeOH in CH₂Cl₂) to give *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (22.1 g, 0.057 mol, 61%) as a colorless oil.

ESI MS *m/e* 386 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.85 (d, *J* = 8.0 Hz, 1 H), 7.47 (t, *J* = 8.4 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.00 (t, *J* = 7.6 Hz, 1 H), 6.60 (brs, 1 H), 6.18 (brs, 1 H), 3.89-3.88 (m, 1 H), 3.39 (brs, 1 H), 3.19 (s, 6 H), 1.77-1.71 (m, 2 H), 1.68-1.52 (m, 6 H), 1.38 (s, 9 H).

Step D: Synthesis of *cis*-*N*²-(4-amino-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazolin-2,4-diamine.

Using the procedure for the step C of example 2338, the title compound was obtained.

ESI MS *m/e* 286 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.84 (d, *J* = 8.4 Hz, 1 H), 7.45 (t, *J* = 6.8 Hz, 1 H), 7.26 (d, *J* = 8.4 Hz, 1 H), 6.99 (t, *J* = 7.6 Hz, 1 H), 6.20 (brs, 1 H), 3.90-3.89 (m, 1 H), 3.18 (s, 6 H), 2.79 (s, 1 H), 1.74-1.71 (m, 2 H), 1.57-1.41 (m, 8 H).

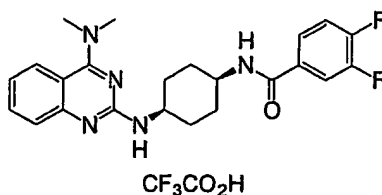
Step E: Synthesis of *cis*-*N*²-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

To a solution of *cis*-*N*²-(4-amino-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazolin-2,4-diamine (31.4 mg, 0.11 mmol) in MeOH (0.5 mL) was added 3,5-dichlorobenzaldehyde (17.5 mg, 0.10 mmol). The mixture was stirred at ambient temperature for 0.5 hr and sodium triacetoxyborohydride (85 mg, 0.40 mmol) was added. The mixture was stirred for overnight and the reaction was quenched with 50% DMSO in water (1.0 mL). The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-*N*²-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (23 mg, 0.041 mmol, 37%) as a white

solid.

ESI MS m/e 444 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 13.55 (s, 1 H), 8.90 (brs, 3 H), 8.17 (d, $J = 8.0$ Hz, 1 H), 7.79 (t, 7.6 Hz, 1 H), 7.68 (s, 1 H), 7.61 (s, 2 H), 7.41 (d, $J = 7.6$ Hz, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 4.23 (s, 2 H), 4.07 (s, 1 H), 3.48 (s, 6 H), 2.00-1.92 (m, 4 H), 1.82-1.74 (m, 4 H).

Example 2342

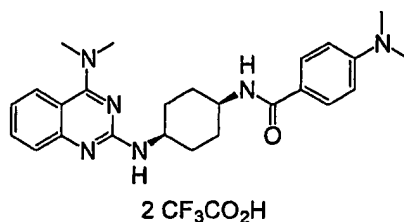


***cis*-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.**

Step A: Synthesis of *cis*-N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.

Using the procedure for the step A of example 2333, the title compound was obtained.

ESI MS m/e 426 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 12.46 (brs, 1 H), 8.36 (s, 1 H), 8.15 (d, $J = 8.0$ Hz, 1 H), 7.97 (brs, 1 H), 7.94-7.89 (m, 1 H), 7.77-7.73 (m, 2 H), 7.56-7.49 (m, 1 H), 7.41 (brs, 1 H), 7.36 (t, $J = 7.6$ Hz, 1 H), 4.07 (m, 1 H), 3.87 (m, 1 H), 3.47 (brs, 6 H), 1.89 (m, 2 H), 1.74 (m, 6 H).

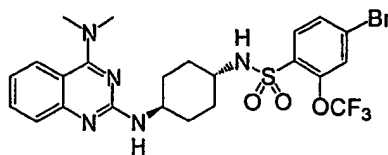
Example 2343

***cis*-4-Dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid**

Step A: Synthesis of *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid.

To a solution of 4-dimethylaminobenzoic acid (16.5 mg, 0.10 mmol) in DMF (0.5 mL) were added HATU (45.6 mg, 0.12 mmol), diisopropylethylamine (34.8 μ L, 0.20 mmol), and *cis*-*N*²-(4-amino-cyclohexyl)-*N*⁴,*N*⁴-dimethyl-quinazolin-2,4-diamine obtained in step D of example 2341 (28.5 mg, 0.10 mmol) and stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.5 mL) and purified by preparative HPLC. The pure fractions combined and lyophilized to give *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid (34.1 mg, 0.052mmol, 52%) as a white solid.

ESI MS *m/e* 433 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.73 (s, 1 H), 8.34 (s, 1 H), 8.16 (d, *J* = 8.0 Hz, 1 H), 7.78-7.70 (m, 4 H), 7.43 (d, *J* = 7.6 Hz, 1 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 6.67 (d, *J* = 8.8 Hz, 2 H), 4.05 (m, 1 H), 3.86 (m, 1 H), 3.47 (s, 6 H), 2.95 (s, 3 H), 2.53 (s, 3 H), 1.91 (m, 2 H), 1.75-1.72 (m, 6 H).

Example 2344

***trans*-4-Bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide**

Step A: Synthesis of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.

To a solution of *trans*-1,4-diamino-cyclohexane (10 g, 0.088 mol) in 1,4-dioxane (400 mL) was added a solution of (Boc)₂O (4.78 g, 0.022 mol) in 1,4-dioxane (100 mL) over 30 min. The mixture was stirred at ambient temperature for overnight and then the dioxane was removed in vacuo. The resulting precipitate was dissolved in H₂O (500 mL) and left to sit for 1 hour. During this time, the di-Boc-protected diamino-cyclohexane fell out as a white crystalline precipitate. This was subsequently filtered from the aqueous solvent. The aqueous layer was extracted with EtOAc (three times). The organic layers were combined and washed with H₂O. The organic layer was dried over MgSO₄ and concentrated to give *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (4 g, 0.019 mol, 85%).

ESI MS *m/e* 215 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 6.63 (d, *J* = 8.0 Hz, 1 H), 3.11-3.09 (m, 1 H), 2.44-2.37 (m, 1 H), 1.70-1.67 (m, 4 H), 1.41-1.31 (m, 11 H), 1.20-0.95 (m, 4 H).

Step B: Synthesis of *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.

To a solution of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (1 g, 0.0047 mol) in CH₂Cl₂ were added diisopropylethylamine (1.63 mL, 0.0093 mol) and 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (1.03 mL, 0.0051 mol). The reaction mixture was stirred at ambient temperature for 1 hr and then washed with water. The aqueous layer was extracted with CH₂Cl₂ (twice), the organic layers were combined, dried over MgSO₄, and concentrated. The resulting precipitate was recrystallized with CH₂Cl₂ and hexanes to give *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (2.39 g, 0.0046 mol, 99%).

ESI MS *m/e* 517 M + H⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.99 (d, *J* = 7.6 Hz, 1 H), 7.85 (d, *J* = 8.0 Hz, 1 H), 7.79-7.77 (m, 1 H), 6.67 (d, *J* = 8.0 Hz, 1 H), 3.14-2.94 (m, 2 H), 1.70-1.60 (m, 4 H), 1.34 (s, 9 H), 1.30-1.18 (m, 2 H), 1.14-1.03 (m, 2 H).

Step C: Synthesis of *trans*-*N*-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.

Using the procedure for the step C of example 2338, the title compound was obtained.

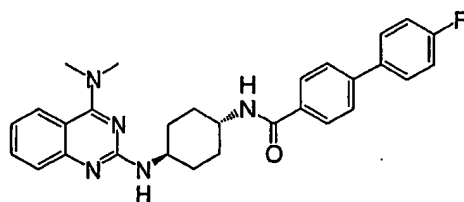
ESI MS m/e 417/419 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.85 (d, $J = 8.4$ Hz, 1 H), 7.79-7.76 (m, 3 H), 3.32 (brs, 2 H), 3.03-2.95 (m, 1 H), 2.41-2.36 (m, 1 H), 1.67-1.57 (m, 4 H), 1.28-1.18 (m, 2 H), 0.99-0.89 (m, 2 H).

Step D: Synthesis of *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide.

To a solution of *trans*-*N*-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide (100 mg, 0.24 mmol) in 2-propanol (0.5 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (54.7 mg, 0.26 mmol). The mixture was heated using a Smith Microwave Synthesizer at 170 °C for 15 min. The mixture was concentrated and the residue was purified by chromatography (2% to 4% 2 M $NH_3/MeOH$ in CH_2Cl_2) to give *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide (42 mg, 0.71 mmol, 30%) as a white solid.

ESI MS m/e 588/590 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 8.02 (d, $J = 7.6$ Hz, 1 H), 7.88 (d, $J = 8.4$ Hz, 1 H), 7.82-7.77 (m, 3 H), 7.45-7.41 (m, 1 H), 7.25-7.41 (m, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 6.37 (brs, 1 H), 3.68-3.67 (m, 1 H), 3.16 (s, 6 H), 3.09-3.02 (m, 1 H), 1.89-1.86 (m, 2 H), 1.69-1.67 (m, 2 H), 1.40-1.17 (m, 4 H).

Example 2345



***trans*-4'-Fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.**

Step A: Synthesis of 4'-fluoro-biphenyl-4-carboxylic acid.

To a solution of 4-bromobenzoic acid (5 g, 0.025 mol) in THF (150 mL) under an

atmosphere of argon were added tetrakis(triphenylphosphine) palladium(0) (862 mg, 0.75 mmol), 2 M aqueous Na_2CO_3 (30 mL), and a solution 4-fluorophenylboronic acid (3.48 g, 0.025 mol) in a minimal amount of ethanol (~10 mL). The resulting reaction mixture was stirred at reflux under an argon atmosphere for overnight. The reaction mixture was cooled to ambient temperature and acidified with addition of 1 M HCl aqueous. The aqueous layer was extracted with Et_2O (three times). The organic layers were combined, dried over MgSO_4 , filtered and concentrated. The resulting precipitate was crystallized in Et_2O and hexane to give 4'-fluoro-biphenyl-4-carboxylic acid (4.4 g, 0.020 mol, 82%) as a white solid.

^1H NMR (400 MHz, DMSO-d_6) δ 12.96 (s, 1 H), 8.00-7.98 (m, 2 H), 7.78-7.75 (m, 4 H), 7.34-7.31 (m, 2 H).

Step B: Synthesis of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.

Using the procedure for the step D of example 2344, the title compound was obtained.

ESI MS m/e 386 $\text{M} + \text{H}^+$; ^1H NMR (400 MHz, DMSO-d_6) δ 7.83 (d, $J = 8.0$ Hz, 1 H), 7.46 (t, $J = 6.8$ Hz, 1 H), 7.27-7.25 (m, 1 H), 6.99 (t, $J = 7.2$ Hz, 1 H), 6.71 (d, $J = 8.4$ Hz, 1 H), 6.38 (brs, 1 H), 3.72 (m, 1 H), 3.17 (s, 6 H), 1.92-1.90 (m, 2 H), 1.79-1.76 (m, 2 H), 1.37 (s, 9 H), 1.34-1.23 (m, 4 H).

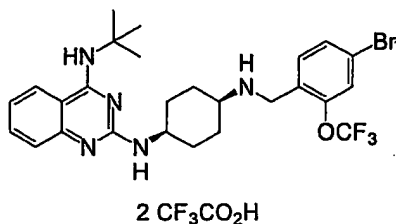
Step C: Synthesis of *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.

To a solution of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (0.76 g, 0.20 mmol) in CH_2Cl_2 (20 mL) was added TFA (304 μL , 0.39 mmol). The solution was stirred at ambient temperature for 4 hr. The resulting mixture was concentrated and the residue was dissolved in CH_2Cl_2 . The organic layer was washed with a dilute aqueous NaOH and aqueous NaHCO_3 solution. The aqueous layer was extracted with CH_2Cl_2 (twice) and the organic layers combined, dried over MgSO_4 , and concentrated. To a solution of the residue (0.1 g) and 4'-fluoro-biphenyl-4-carboxylic acid (76 mg, 0.35 mmol) in CH_2Cl_2 were added HOAt (62 mg, 0.46 mmol), WSC $\cdot\text{HCl}$ (87 mg, 0.46 mmol), and diisopropylethylamine (31 μL , 0.18 mmol). The mixture was stirred for 1 hr at ambient temperature and the reaction was quenched with

water. The aqueous layer was extracted with CH_2Cl_2 (twice). The organic layers were combined, dried over MgSO_4 , concentrated and the residue purified by column chromatography (silica gel, 2% to 4% 2 M NH_3/MeOH in CH_2Cl_2) to give *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide (35 mg, 0.072, 21%) as a white solid.

ESI MS m/e 484 $M + H^+$; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.30 (brs, 1 H), 8.12 (brs, 2 H), 7.92 (d, $J = 8.4$ Hz, 2 H), 7.77-7.72 (m, 5 H), 7.44 (brs, 1 H), 7.34-7.28 (m, 3 H), 3.82 (brs, 2 H), 3.47 (brs, 6 H), 2.04 (m, 2 H), 1.94 (m, 2 H), 1.54-1.48 (m, 4 H).

Example 2346



cis- N^2 -[4-(4-Bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]- N^4 -*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

Step A: Synthesis of *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine.

To a solution of 2,4-dichloro-quinazoline obtained in step B of example 1 (4 g, 20 mmol) in THF (50 mL) were added *tert*-butyl amine (2.15 mL, 20.5 mmol) and diisopropylethylamine (3.5 mL, 21 mmol). The mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated and the residue was dissolved in EtOAc. The organic layer was washed with water, dried over Na_2SO_4 , and filtered. The mixture was concentrated to give *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine as a white solid (3 g, 64%).

ESI MS m/e 236 $M + H^+$; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.40 (d, $J = 8.4$ Hz, 1 H), 7.75-7.36 (m, 2 H), 7.58 (d, $J = 8.4$ Hz, 1 H), 7.48 (t, $J = 7.2$ Hz, 1 H), 1.52 (s, 9 H).

Step B: Synthesis of *cis*- N^2 -(4-amino-cyclohexyl)- N^4 -*tert*-butyl-quinazoline-2,4-diamine.

To a suspension of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (122

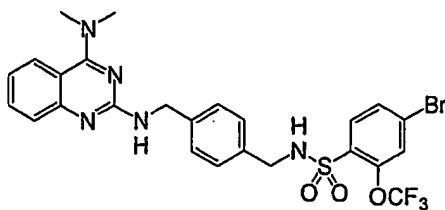
mg, 0.57 mmol) in 2-propanol (2 mL) were added *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine (100 mg, 0.42 mmol) and diisopropylethylamine (180 μ L, 1 mmol) and the mixture was heated at 170 °C for 1 hr using a Smith Microwave Synthesizer. The resulting solution was concentrated and purified by column chromatography (silica gel, 3% MeOH in CH₂Cl₂) to give [4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (112 mg, 65%) as a yellow solid. To a suspension of *cis*-[4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (95 mg, 0.23 mmol) in CH₂Cl₂ (3 mL) was added trifluoroacetic acid (2 mL) dropwise. The reaction mixture was stirred at ambient temperature for 2 hr. The solution was concentrated, alkalized with saturated aqueous NaHCO₃ and 1 M aqueous sodium hydroxide (pH = 9), and the aqueous layer was extracted with CH₂Cl₂ (three times). The combined organic layer was dried over MgSO₄, filtered, and concentrated. The solid was collected by filtration to give *cis*-N²-(4-amino-cyclohexyl)-N⁴-*tert*-butyl-quinazoline-2,4-diamine (44.6 mg, 53%) as a yellow solid.

ESI MS *m/e* 314 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 7.48 (t, *J* = 6.8 Hz, 1 H), 7.38 (m, 2 H), 7.04 (t, *J* = 8.0 Hz, 1 H), 5.42 (brs, 1 H), 4.15 (m, 1 H), 2.85 (m, 1 H), 1.2-1.9 (m, 17 H).

Step C: Synthesis of *cis*-N²-[4-(4-bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]-N⁴-*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.

Using the procedure for the step C of example 2341, the title compound was obtained.

ESI MS *m/e* 566 M + H⁺; ¹H NMR (400 MHz, CDCl₃) δ 9.36 (d, *J* = 8.0 Hz, 1 H), 7.67-7.64 (m, 2 H), 7.53-7.48 (m, 3 H), 7.43 (s, 1 H), 7.33 (m, 1 H), 6.17 (s, 1 H), 4.45 (m, 1 H), 4.28 (s, 2 H), 3.35 (m, 1 H), 2.14-1.6 (m, 17 H).

Example 2347

4-Bromo-N-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide

Step A: Synthesis of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester.

Using the procedure for the step D of example 2330, the title compound was obtained.

ESI MS m/e 377 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 8.38 (brs, 1 H), 8.08 (brs, 1 H), 7.70 (brs, 1 H), 7.47 (brs, 1 H), 7.36 (t, $J = 6.2$ Hz, 1 H), 7.30 (d, $J = 8.0$ Hz, 3 H), 7.16 (d, $J = 7.6$ Hz, 2 H), 4.60 (d, $J = 6.4$ Hz, 2 H), 4.07 (d, $J = 6.0$ Hz, 2 H), 3.39 (s, 6 H), 1.37 (s, 9 H).

Step B: Synthesis of N^2 -(4-aminomethyl-benzyl)- N^1,N^4 -dimethyl-quinazoline-2,4-diamine hydrochloride.

To a cooled solution of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester (3.90 g, 9.57 mmol) in MeOH was added 1 M HCl in Et₂O (67.0 ml, 67.0 mmol) and the solution was stirred for overnight. The resulting mixture was concentrated to give N^2 -(4-aminomethyl-benzyl)- N^1,N^4 -dimethyl-quinazoline-2,4-diamine hydrochloride as a white crystalline solid (3.48 g, 95.6%).

ESI MS m/e 308.2 $M + H^+$; 1H NMR (400 MHz, CD₃OD) δ 8.16 (d, $J = 7.2$ Hz, 1 H), 7.75 (brs, 1 H), 7.48 (m, 5 H), 7.39 (brs, 1 H), 4.76 (s, 2 H), 4.12 (s, 2 H), 3.51 (m, 6 H).

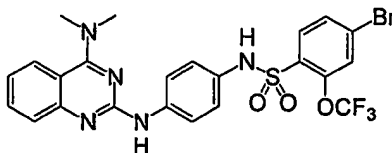
Step C: Synthesis of 4-bromo-N-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide.

A solution of N^2 -(4-aminomethyl-benzyl)- N^1,N^4 -dimethyl-quinazoline-2,4-diamine hydrochloride (50.0 mg, 0.131 mmol), 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (53.3 mg, 0.157 mmol) and diisopropylethylamine (91 μ l, 0.524 mmol) in 2-

propanol (1.5 mL) was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated, and the residue was purified by column chromatography (silica gel, 10% MeOH in CH₂Cl₂) to give 4-bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide as a white crystalline compound (40 mg, 50%).

ESI MS *m/e* 612 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.51 (t, *J* = 6.4 Hz, 1 H), 8.06 (brs, 1 H), 7.76-7.67 (m, 4 H), 7.54-7.41 (m, 2 H), 7.24 (d, *J* = 7.6 Hz, 3 H), 7.14 (d, *J* = 8.0 Hz, 2 H), 4.56 (d, *J* = 6.0 Hz, 2 H), 4.08 (d, *J* = 6.0 Hz, 2 H), 3.36 (s, 6 H).

Example 2348



4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide

Step A: Synthesis of (4-amino-phenyl)-carbamic acid *tert*-butyl ester.

Using the procedure for the step A of example 2344, the title compound was obtained.

ESI MS *m/e* 209 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.75 (s, 1 H), 7.03 (d, *J* = 7.6 Hz, 2 H), 6.43 (dt, *J* = 9.5, 2.7 Hz, 2 H), 4.71 (s, 2 H), 1.43 (s, 9 H).

Step B: Synthesis of *N*²-(4-amino-phenyl)-*N*⁴,*N*⁴-dimethyl-quinazoline-2,4-diamine hydrochloride.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.5 g, 2.6 mmol) and (4-amino-phenyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.6 mmol) in CH₂Cl₂ (2 mL) was heated by Smith Synthesizer at 130 °C for 20 min. The mixture was concentrated to give [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-carbamic acid *tert*-butyl ester as a pale yellow solid (0.86 g, 87%). The reaction was repeated six times, and the total product combined was 8.5 g. To a solution of above product (8.5 g, 22.4 mmol) in MeOH (250 mL) was added 4 M HCl in dioxane (8.4 ml,

33.6 mmol) dropwise, and the mixture was stirred at ambient temperature for overnight. The mixture was concentrated to give *N*²-(4-amino-phenyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride as a pale pink solid (6.2 g, 87.5%).

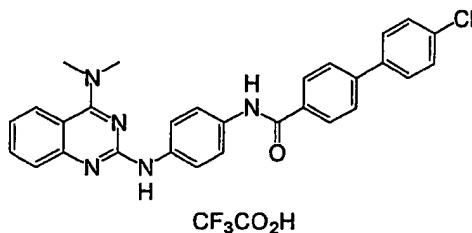
ESI MS *m/e* 280 *M* + *H*⁺; ¹H NMR (400 MHz, D₂O) δ 7.84 (d, *J* = 8.8 Hz, 1 H), 7.54 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.46 (dt, *J* = 9.5, 2.7 Hz, 2 H), 7.27-7.16 (m, 4 H), 3.35 (b, 3 H), 3.12 (b, 3 H).

Step C: Synthesis of 4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide.

Using the procedure for the step C of example 2347, the title compound was obtained.

ESI MS *m/e* 584 *M* + *H*⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.27 (brs, 1 H), 9.14 (brs, 1 H), 7.98 (d, *J* = 8.4 Hz, 1 H), 7.80-7.71 (m, 5 H), 7.60-7.56 (m, 1 H), 7.44 (d, *J* = 8.4 Hz, 1 H), 7.15 (t, *J* = 7.4 Hz, 1 H), 6.95 (d, *J* = 16.8 Hz, 2 H), 9.29 (s, 6 H).

Example 2349



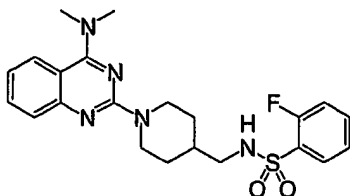
4'-Chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid

Synthesis of 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid.

A solution of *N*²-(4-amino-phenyl)-*N*¹,*N*¹-dimethyl-quinazoline-2,4-diamine hydrochloride obtained in step B of example 2348 (81.6 mg, 0.258 mmol), 4'-chloro-biphenyl-4-carboxylic acid (50.0 mg, 0.215 mmol), HATU (106 mg, 0.280 mmol), and diisopropylethylamine (150 μL, 0.860 mmol), in CH₂Cl₂ (2 mL) was stirred at ambient temperature for overnight, and the mixture was concentrated. The residue was purified by HPLC to give 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid as a white solid (10 mg, 9 %).

ESI MS m/e 494 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 10.33 (s, 1 H), 8.17 (d, J = 8.0 Hz, 1 H), 8.80 (d, J = 8.8 Hz, 2 H), 7.85-7.75 (m, 7 H), 7.63-7.53 (m, 6 H), 7.36 (t, J = 7.6 Hz, 1 H), 3.46 (s, 6 H).

Example 2350



***N*-[1-(4-Dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide**

Step A: Synthesis of *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide.

To a solution of 4-aminomethyl-piperidine-1-carboxylic acid *tert*-butyl ester (60 mg, 0.28 mmol) and diisopropylethylamine (49 mL, 0.28 mmol) in CH_2Cl_2 (2 mL) was added 2-fluorobenzenesulfonyl chloride (54 mg, 0.28 mmol) and the mixture was stirred at ambient temperature for 18 hr. To the resulting mixture was added trifluoroacetic acid (0.70 mL) and stirred at ambient temperature for 18 hr. The reaction mixture was concentrated and neutralized with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with EtOAc, and the organic layer was concentrated to give 2-fluoro-*N*-piperidin-4-ylmethyl-benzenesulfonamide as a pale yellow solid. To a solution of above solid (0.076 g, 0.28 mmol) and diisopropylethylamine (0.072 mL, 0.42 mmol) in 2-propanol (3 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.044 g, 0.21 mmol) and the resulting mixture was stirred at 100 °C for 18 hr. The mixture was concentrated, and the residue was purified by column chromatography (silica gel, 5% MeOH in CH_2Cl_2) to give *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluoro-benzenesulfonamide as a pale yellow solid (0.024 g, 26%).

ESI MS m/e 444 $M + H^+$; 1H NMR (400 MHz, DMSO- d_6) δ 7.98 (m, 1 H), 7.86 (m, 1 H), 7.77 (m, 1 H), 7.67 (m, 1 H), 7.47-7.29 (m, 4 H), 7.02 (m, 1 H), 4.69 (m, 2 H), 3.21 (s, 6 H), 2.76 (m, 4 H), 1.66 (m, 3 H), 1.00 (m, 2 H).

Using the procedure for example 2329 and purification by preparative HPLC, the compounds of example 2351 - 2819 were obtained.

Using the procedure for example 2331 and purification by preparative HPLC, the compounds of example 2820 - 2842 were obtained.

Using the procedure for example 2332, the compounds of example 2843 - 3003 were obtained.

Using the procedure for example 2333, the compounds of example 3004 - 3090 were obtained.

Using the procedure for example 2334, the compounds of example 3091 - 3161 were obtained.

Using the procedure for example 2335 and purification by preparative HPLC, the compounds of example 3162 - 3178 were obtained.

Using the procedure for example 2336, the compounds of example 3179 - 3208 were obtained.

Using the procedure for example 2337, the compounds of example 3209 was obtained.

Using the procedure for example 2338, the compounds of example 3210 - 3225 were obtained.

Using the procedure for example 2339, the compounds of example 3226 - 3228 were obtained.

Using the procedure for example 2340, the compounds of example 3229 - 3231 were obtained.

Using the procedure for example 2341, the compounds of example 3232 - 3393 were obtained.

Using the procedure for example 2342, the compounds of example 3394 - 3472 were obtained.

Using the procedure for example 2343, the compounds of example 3473 - 3527 were obtained.

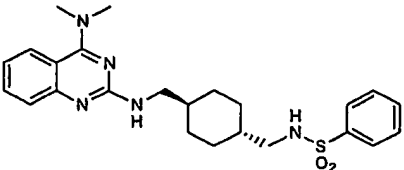
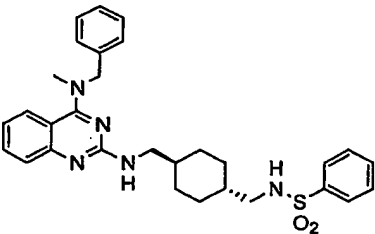
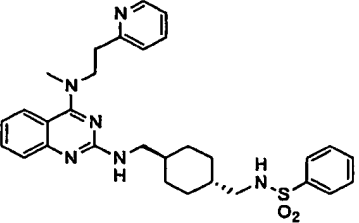
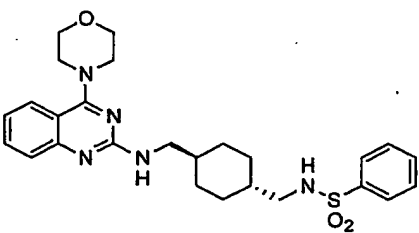
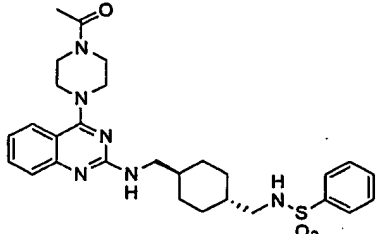
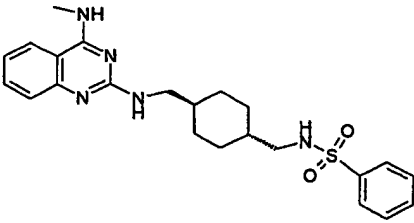
Using the procedure for example 2346, the compounds of example 3528 - 3535 were obtained.

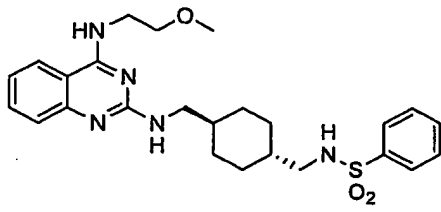
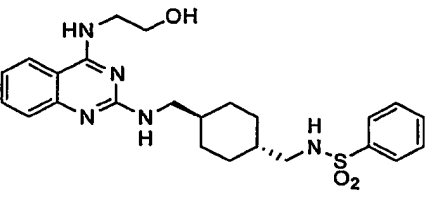
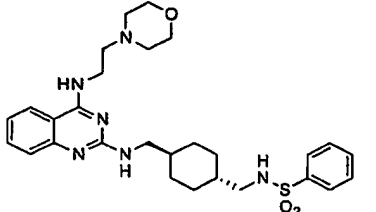
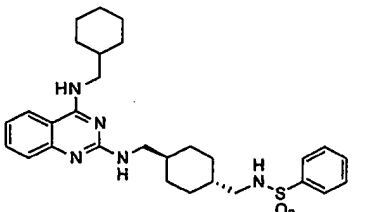
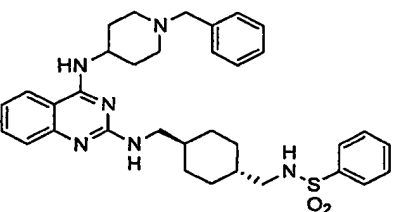
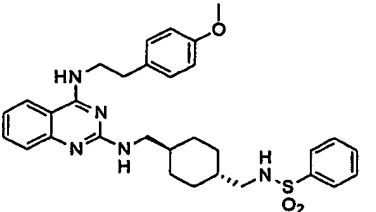
Using the procedure for example 2347 and purification by preparative HPLC, the compounds of example 3536 - 3545 were obtained.

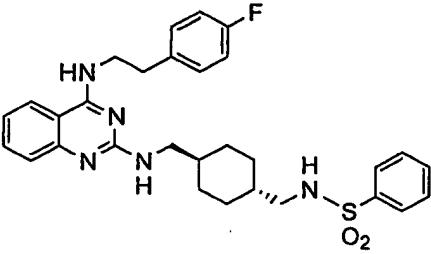
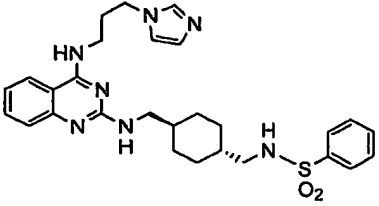
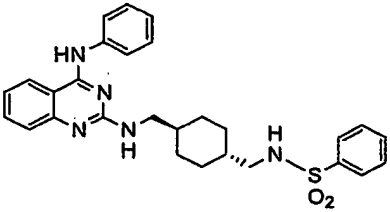
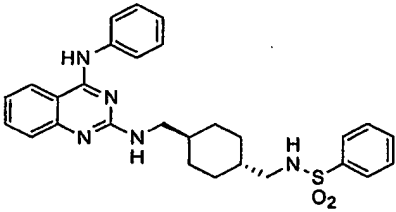
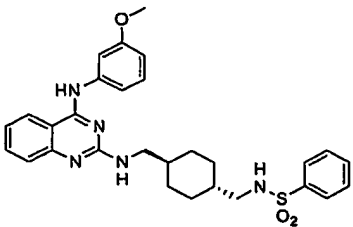
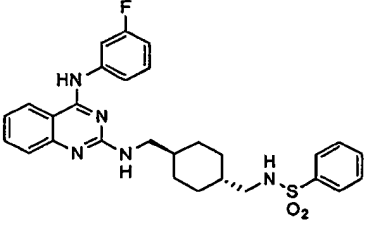
Using the procedure for example 2348 and purification by preparative HPLC, the compounds of example 3546 - 3548 were obtained.

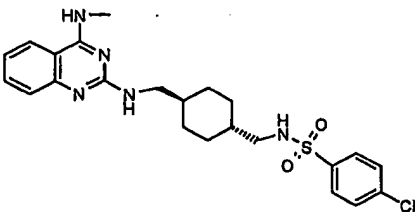
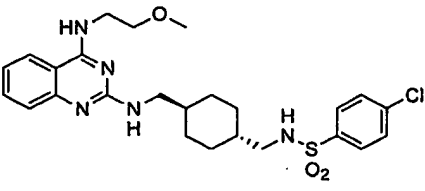
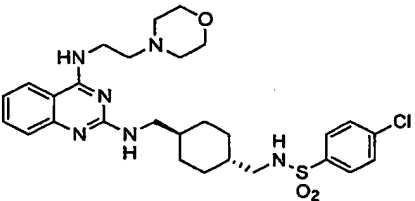
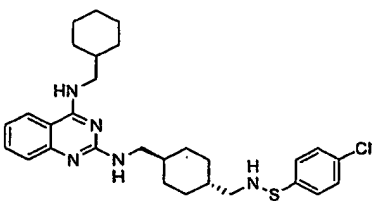
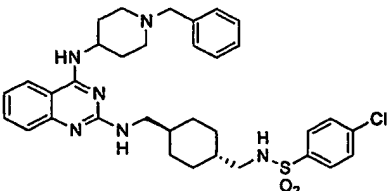
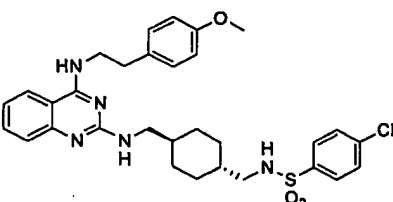
Using the procedure for example 2349, the compounds of example 3549 - 3567 were obtained.

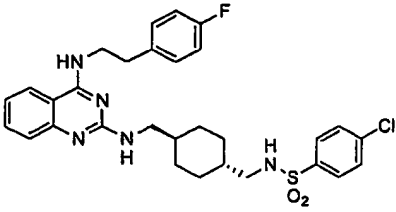
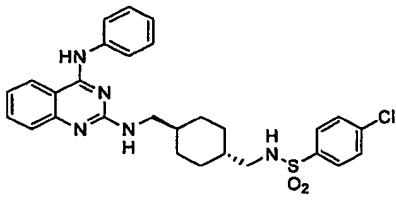
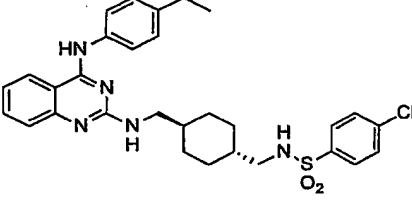
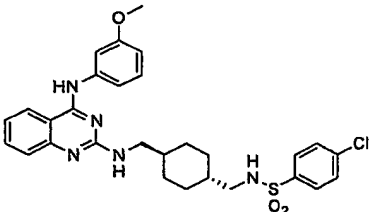
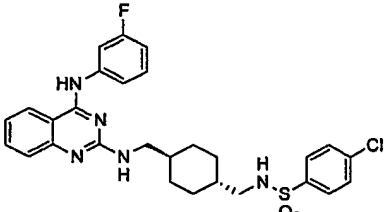
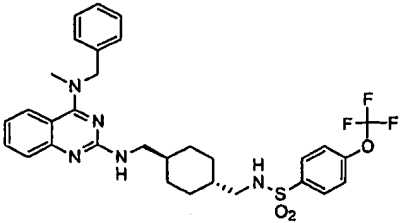
Using the procedure for example 2350 and purification by preparative HPLC, the compounds of example 3568 - 3579 were obtained.

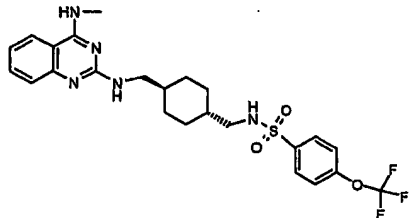
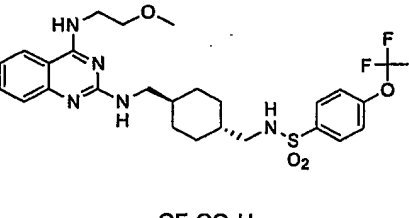
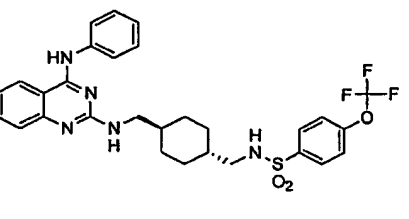
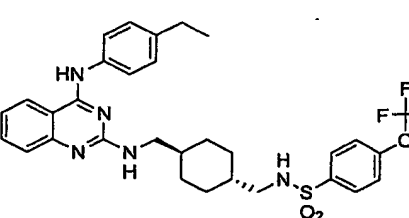
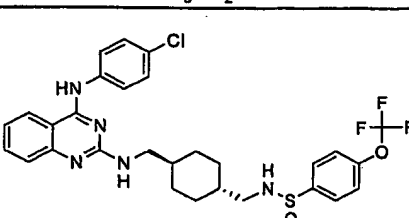
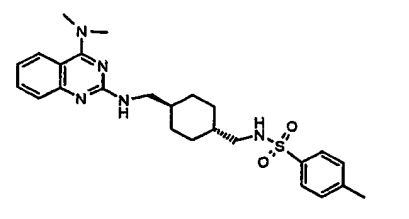
Example No.	Structure	ESI-MS	Retention Time (min)
2351	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.60
2352	 <chem>Cc1ccccc1n2c(c3ccccc3n2)N[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	4.02
2353	 <chem>Cc1cccnc1CN[C@H]2CCCC[C@H]2NS(=O)(=O)c3ccccc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	545.4 (M + H)	3.05
2354	 <chem>C1CCN(C1)c2nc3ccccc3n2N[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.49
2355	 <chem>CC(=O)N1CCN(C1)c2nc3ccccc3n2N[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	537.4 (M + H)	3.24
2356	 <chem>CN1=NC2=CC=CC=C2N=CN1[C@H]3CCCC[C@H]3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.47

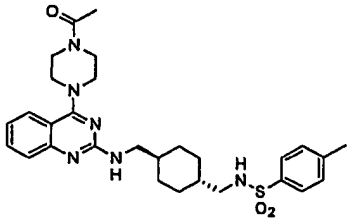
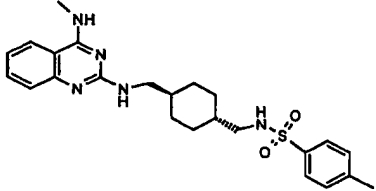
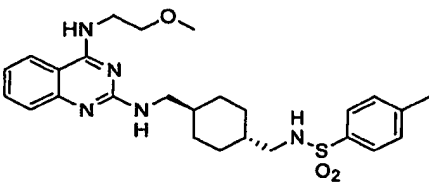
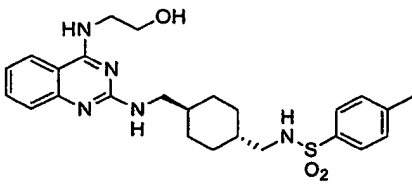
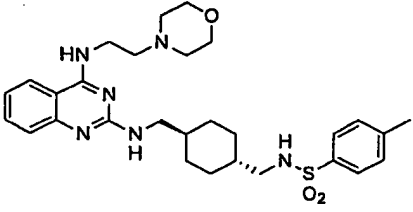
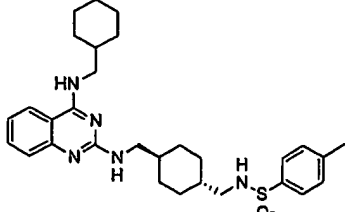
Example No.	Structure	ESI-MS	Retention Time (min)
2357	 $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	3.49
2358	 $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	3.20
2359	 $2\text{CF}_3\text{CO}_2\text{H}$	539.4 (M + H)	3.12
2360	 $\text{CF}_3\text{CO}_2\text{H}$	522.2 (M + H)	4.22
2361	 $2\text{CF}_3\text{CO}_2\text{H}$	599.0 (M + H)	3.48
2362	 $\text{CF}_3\text{CO}_2\text{H}$	560.2 (M + H)	3.99

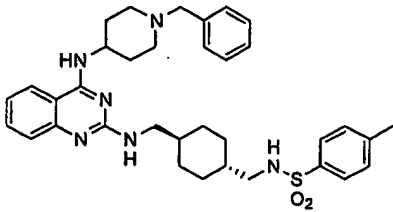
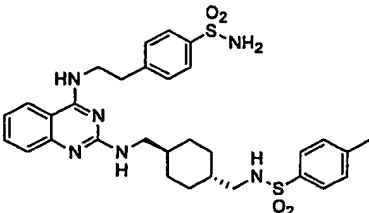
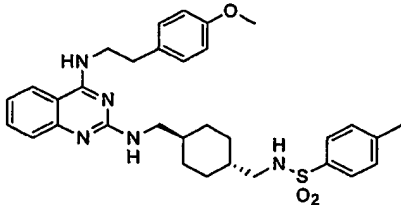
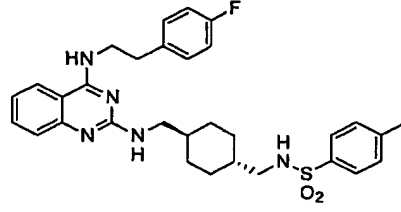
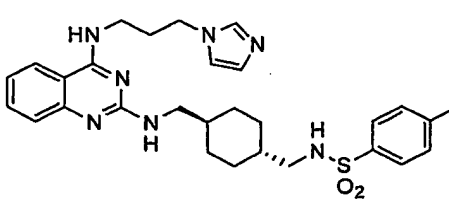
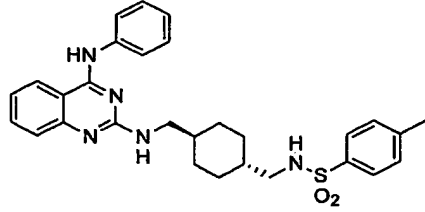
Example No.	Structure	ESI-MS	Retention Time (min)
2363		548.4 (M + H)	4.06
2364	 2CF ₃ CO ₂ H	534.0 (M + H)	3.11
2365	 CF ₃ CO ₂ H	502.4 (M + H)	3.81
2366	 CF ₃ CO ₂ H	530.2 (M + H)	4.04
2367	 CF ₃ CO ₂ H	532.4 (M + H)	3.85
2368	 CF ₃ CO ₂ H	520.2 (M + H)	3.86

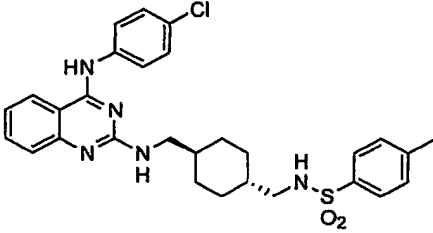
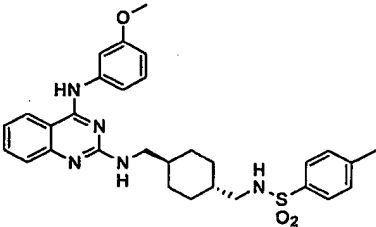
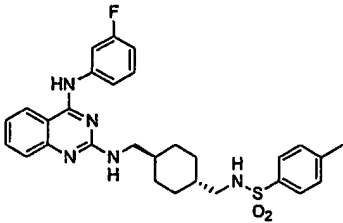
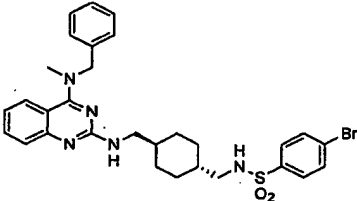
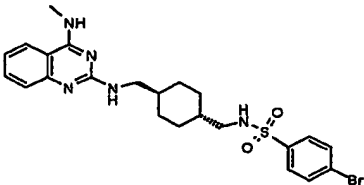
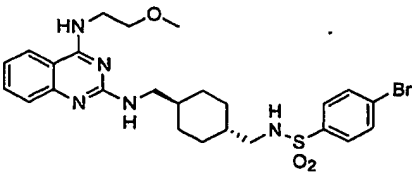
Example No.	Structure	ESI-MS	Retention Time (min)
2369	 <chem>CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.2 (M + H)	3.72
2370	 <chem>COCCN1C=NC2=CC=CC=C2N1CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.2 (M + H)	3.71
2371	 <chem>C1CCN(C1)CCN2C=NC3=CC=CC=C3N2CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	573.2 (M + H)	3.15
2372	 <chem>C1CCCCC1CN2C=NC3=CC=CC=C3N2CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.2 (M + H)	4.38
2373	 <chem>C1CCN(C1)CCN2C=NC3=CC=CC=C3N2CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	633.4 (M + H)	3.48
2374	 <chem>COc1ccc(cc1)CN2C=NC3=CC=CC=C3N2CC1(CCN2C=NC3=CC=CC=C3N2)CC1CCSC(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	594.2 (M + H)	4.23

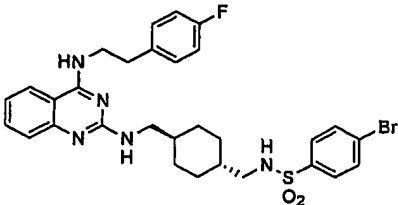
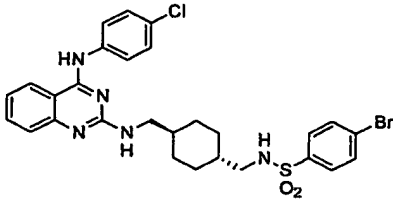
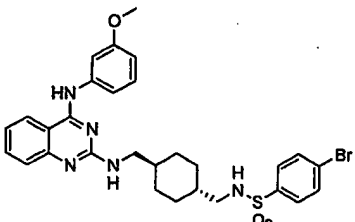
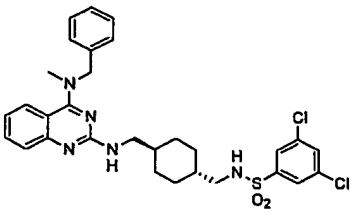
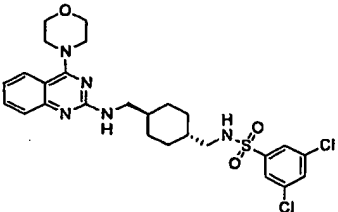
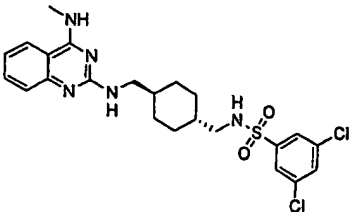
Example No.	Structure	ESI-MS	Retention Time (min)
2375	 <chem>CF3CO2H</chem>	582.4 (M + H)	4.26
2376	 <chem>CF3CO2H</chem>	536.2 (M + H)	4.06
2377	 <chem>CF3CO2H</chem>	564.2 (M + H)	4.32
2378	 <chem>CF3CO2H</chem>	566.4 (M + H)	4.11
2379	 <chem>CF3CO2H</chem>	554.2 (M + H)	4.10
2380	 <chem>CF3CO2H</chem>	614.2 (M + H)	4.26

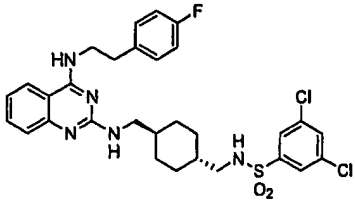
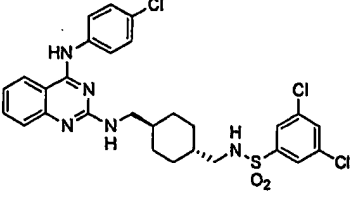
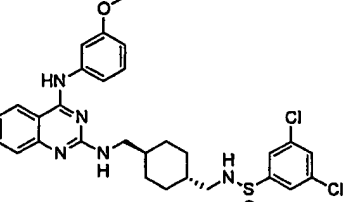
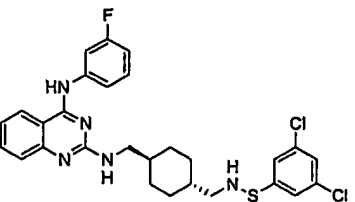
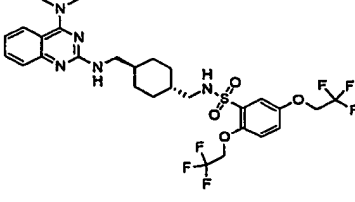
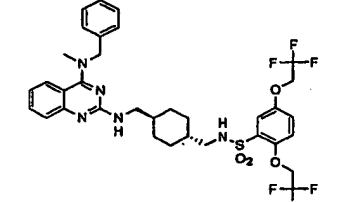
Example No.	Structure	ESI-MS	Retention Time (min)
2381	 <chem>COc1nc2c(ncn2C1CC2CCCCC2NS(=O)(=O)c3ccc(OC(F)(F)F)cc3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.4 (M + H)	3.87
2382	 <chem>COCCNc1nc2c(ncn2C1CC2CCCCC2NS(=O)(=O)c3ccc(OC(F)(F)F)cc3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	568.2 (M + H)	3.87
2383	 <chem>c1ccc(Nc2nc3c(ncn3C1CC2CCCCC2NS(=O)(=O)c4ccc(OC(F)(F)F)cc4)cc2)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	4.18
2384	 <chem>CCc1ccc(Nc2nc3c(ncn3C1CC2CCCCC2NS(=O)(=O)c4ccc(OC(F)(F)F)cc4)cc2)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	614.2 (M + H)	4.45
2385	 <chem>Clc1ccc(Nc2nc3c(ncn3C1CC2CCCCC2NS(=O)(=O)c4ccc(OC(F)(F)F)cc4)cc2)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	620.4 (M + H)	4.32
2386	 <chem>CN1C=NC2=C(N1)C=CC=C2C3CC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.20

Example No.	Structure	ESI-MS	Retention Time (min)
2387	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $\text{CF}_3\text{CO}_2\text{H}$	551.6 (M + H)	2.82
2388	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.06
2389	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.6 (M + H)	3.10
2390	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	2.76
2391	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	553.6 (M + H)	2.40
2392	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=CC=C4S(=O)(=O)N[C@H]5CCCC[C@H]5C6CCN(C)CC6</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.77

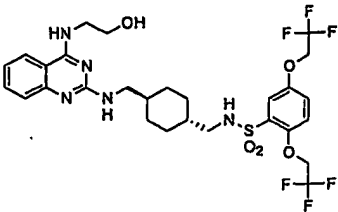
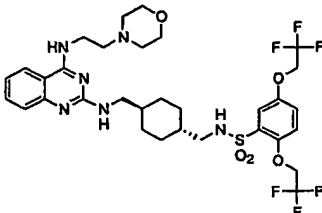
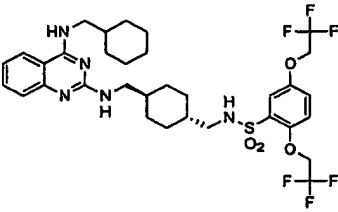
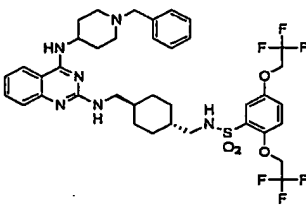
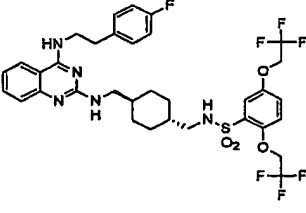
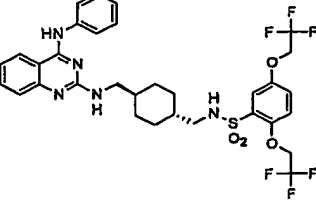
Example No.	Structure	ESI-MS	Retention Time (min)
2393	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C3)NC5=CC=CC=C5C6=CC=CC=C6N6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	613.4 (M + H)	2.74
2394	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C3)NC5=CC=CC=C5C6=CC=C(C=C6)S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	3.06
2395	 <chem>COc1ccc(cc1)NC2=NC3=CC=CC=C3N(C2)NC4=CC=CC=C4C5=CC=CC=C5N5</chem> $\text{CF}_3\text{CO}_2\text{H}$	574.4 (M + H)	3.51
2396	 <chem>Cc1ccc(cc1)S(=O)(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C3)NC5=CC=C(F)C=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	3.59
2397	 <chem>Cc1ccc(cc1)S(=O)(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C3)NC5=CC=CN=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	548.6 (M + H)	2.48
2398	 <chem>Cc1ccc(cc1)S(=O)(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C3)Nc5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.39

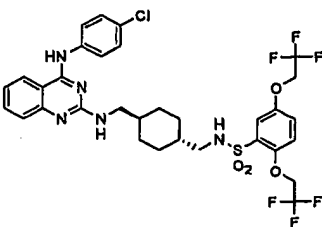
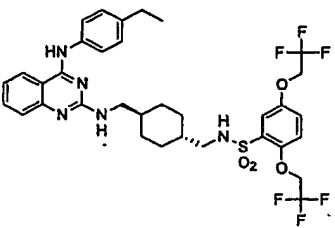
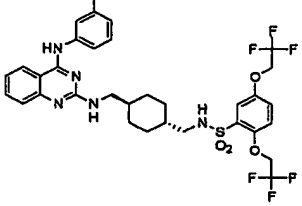
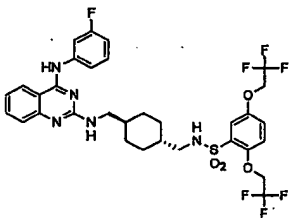
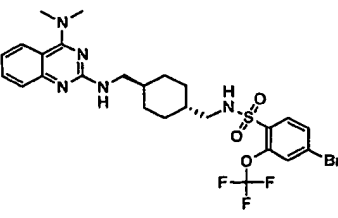
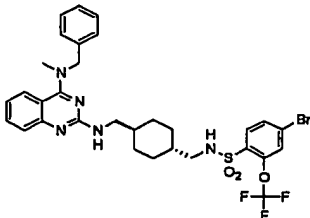
Example No.	Structure	ESI-MS	Retention Time (min)
2399	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3c5ccc(Cl)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.4 (M + H)	3.56
2400	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4cc(OC)cc4N3c5ccc(OC)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.2 (M + H)	3.38
2401	 <chem>CC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3c5ccc(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.0 (M + H)	3.43
2402	 <chem>BrC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	608.2 (M + H)	3.75
2403	 <chem>BrC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	518 (M + H)	3.22
2404	 <chem>BrC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	3.20

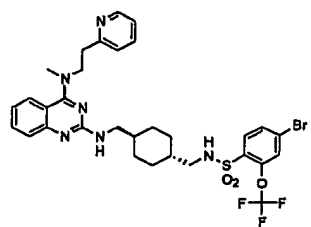
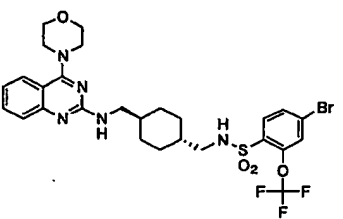
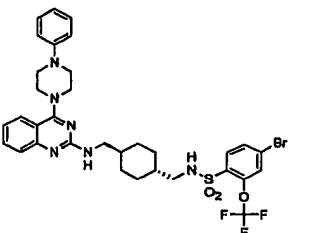
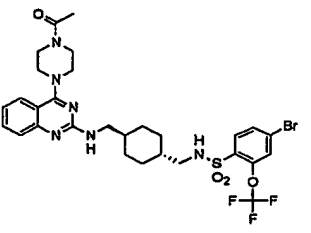
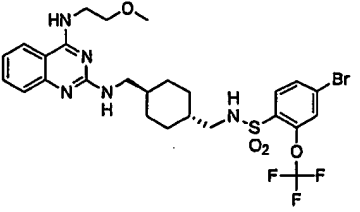
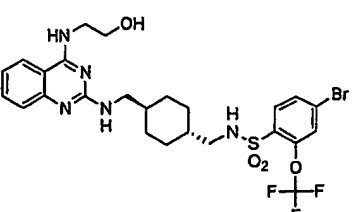
Example No.	Structure	ESI-MS	Retention Time (min)
2405	 $\text{CF}_3\text{CO}_2\text{H}$	626.0 (M + H)	3.76
2406	 $\text{CF}_3\text{CO}_2\text{H}$	614.0 (M + H)	3.72
2407	 $\text{CF}_3\text{CO}_2\text{H}$	610.0 (M + H)	3.57
2408	 $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	3.97
2409	 $\text{CF}_3\text{CO}_2\text{H}$	564.2 (M + H)	3.46
2410	 $\text{CF}_3\text{CO}_2\text{H}$	508.0 (M + H)	3.44

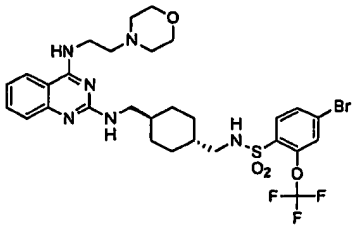
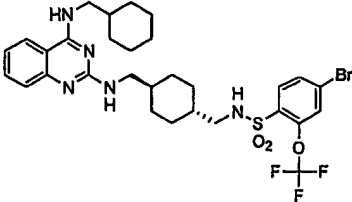
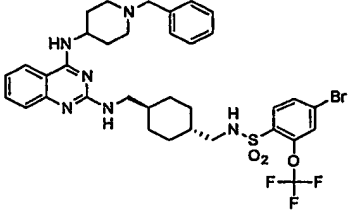
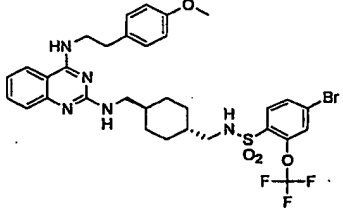
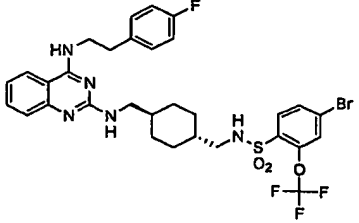
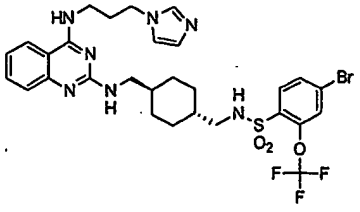
Example No.	Structure	ESI-MS	Retention Time (min)
2411	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(Cl)cc(Cl)c4)C)C(F)(F)F(=O)O</chem>	616.2 (M + H)	3.94
2412	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(Cl)cc(Cl)c4)C)C(F)(F)F(=O)O</chem>	604.2 (M + H)	4.51
2413	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(Cl)cc(Cl)c4)C)C(F)(F)F(=O)O</chem>	600.2 (M + H)	4.32
2414	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(Cl)cc(Cl)c4)C)C(F)(F)F(=O)O</chem>	588.0 (M + H)	4.38
2415	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(F)c(F)c4)C)C(F)(F)F(=O)O</chem>	650.2 (M + H)	4.20
2416	 <chem>CC1(CCN2C(=N1)N(C2)CN(C2)C3CC(C(C3)CSC(=O)(=O)c4cc(F)c(F)c4)C)C(F)(F)F(=O)O</chem>	726.4 (M + H)	4.52

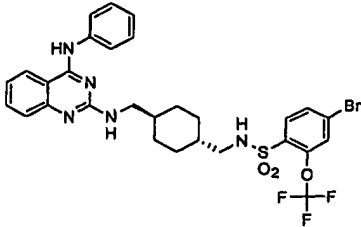
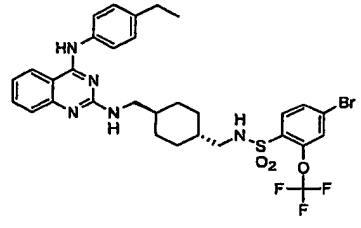
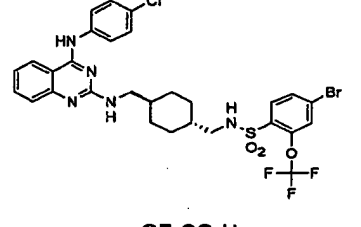
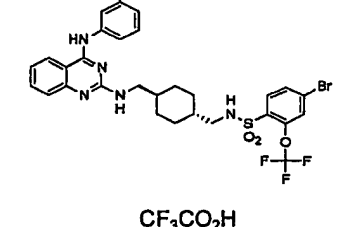
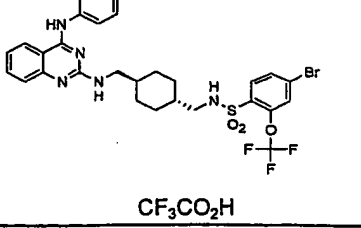
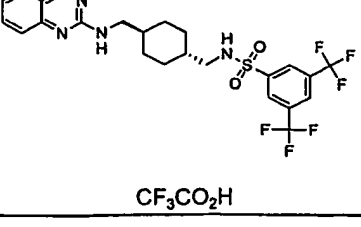
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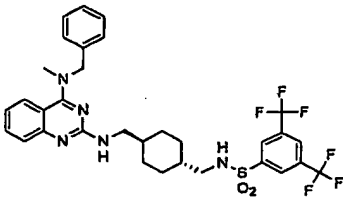
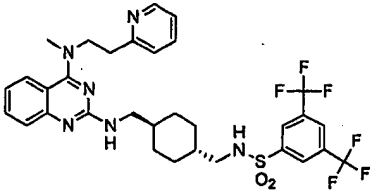
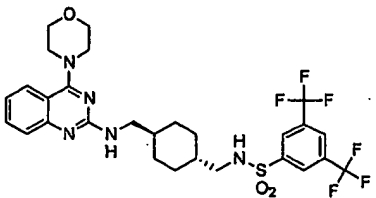
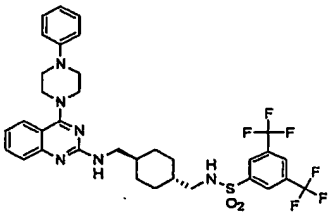
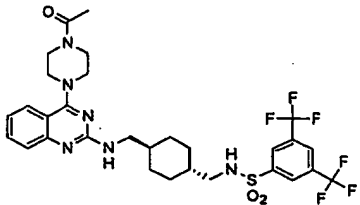
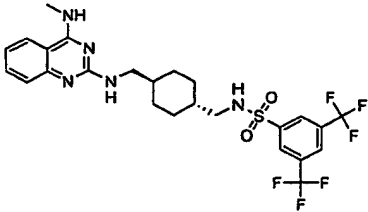
Example No.	Structure	ESI-MS	Retention Time (min)
2423	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	666.0 (M + H)	3.86
2424	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	735.4 (M + H)	3.50
2425	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	718.4 (M + H)	4.64
2426	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	795.6 (M + H)	3.70
2427	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	744.2 (M + H)	4.43
2428	 <chem>CC1(CCN1c2nc3ccccc3n2)C[C@H](C1)NS(=O)(=O)c1cc(OC(F)(F)F)cc(OC(F)(F)F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	698.0 (M + H)	4.26

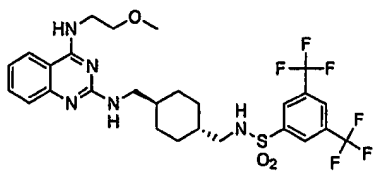
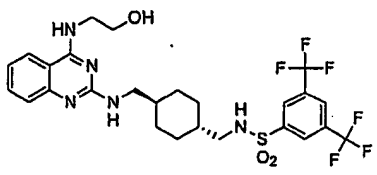
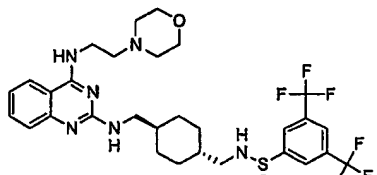
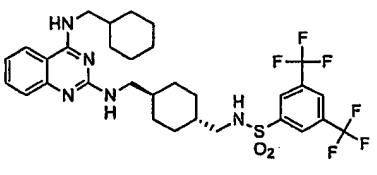
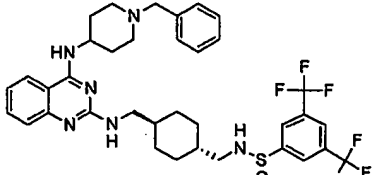
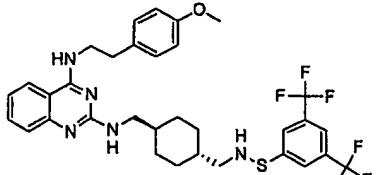
Example No.	Structure	ESI-MS	Retention Time (min)
2429	 <chem>Clc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	732.4 (M + H)	4.37
2430	 <chem>CCc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	726.4 (M + H)	4.52
2431	 <chem>COc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	728.4 (M + H)	4.36
2432	 <chem>Fc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	716.4 (M + H)	4.32
2433	 <chem>CN(C)c1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5Br)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	616.0 (M + H)	4.22
2434	 <chem>CN(CCc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5Br)cc1)</chem> $\text{CF}_3\text{CO}_2\text{H}$	692.0 (M + H)	4.57

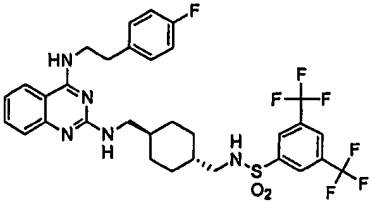
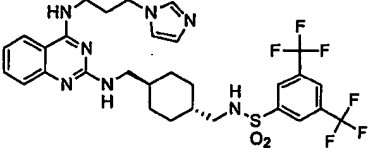
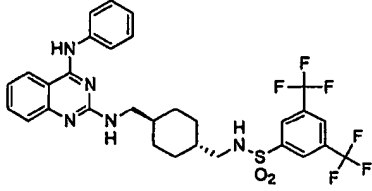
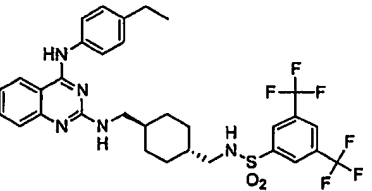
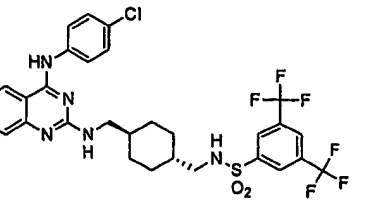
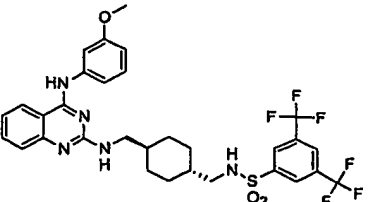
Example No.	Structure	ESI-MS	Retention Time (min)
2435	 $2\text{CF}_3\text{CO}_2\text{H}$	707.2 (M + H)	3.64
2436	 $\text{CF}_3\text{CO}_2\text{H}$	658.2 (M + H)	4.15
2437	 $\text{CF}_3\text{CO}_2\text{H}$	733.2 (M + H)	4.68
2438	 $\text{CF}_3\text{CO}_2\text{H}$	699.2 (M + H)	3.88
2439	 $\text{CF}_3\text{CO}_2\text{H}$	646.4 (M + H)	4.08
2440	 $\text{CF}_3\text{CO}_2\text{H}$	632.4 (M + H)	3.86

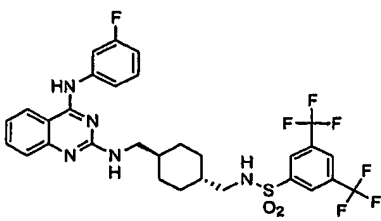
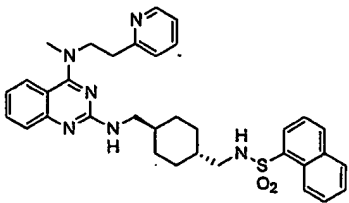
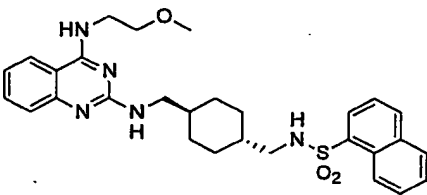
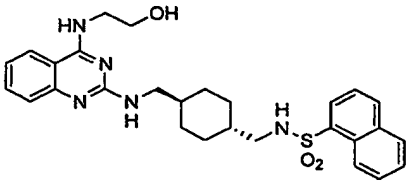
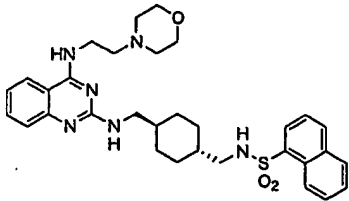
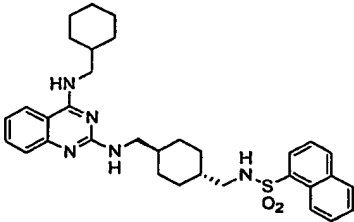
Example No.	Structure	ESI-MS	Retention Time (min)
2441	 $2\text{CF}_3\text{CO}_2\text{H}$	701.4 (M + H)	3.51
2442	 $\text{CF}_3\text{CO}_2\text{H}$	684.2 (M + H)	4.75
2443	 $2\text{CF}_3\text{CO}_2\text{H}$	761.2 (M + H)	3.74
2444	 $\text{CF}_3\text{CO}_2\text{H}$	722.2 (M + H)	4.59
2445	 $\text{CF}_3\text{CO}_2\text{H}$	710.2 (M + H)	4.60
2446	 $2\text{CF}_3\text{CO}_2\text{H}$	696.2 (M + H)	3.53

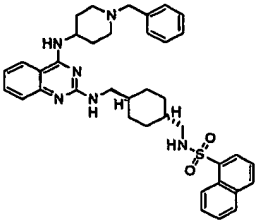
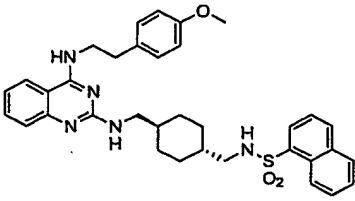
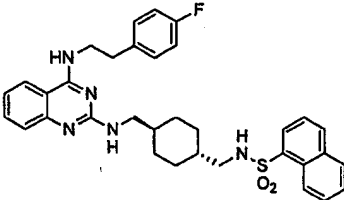
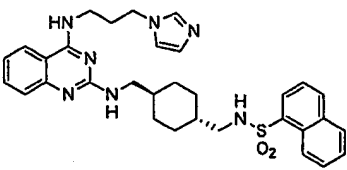
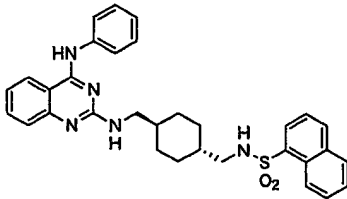
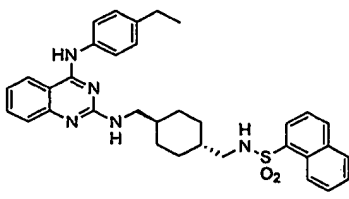
Example No.	Structure	ESI-MS	Retention Time (min)
2447	 <chem>CC1(CCN2C(=N1)N(C2)C3CCCCC3NS(=O)(=O)C4=CC=C(C=C4)OC(F)(F)F)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	664.2 (M + H)	4.39
2448	 <chem>CC1(CCN2C(=N1)N(C2)C3CCCCC3NS(=O)(=O)C4=CC=C(C=C4)OC(F)(F)F)C5=CC=C(C=C5)CC</chem> $\text{CF}_3\text{CO}_2\text{H}$	692.0 (M + H)	4.65
2449	 <chem>ClC1=CC=C(C=C1)N2C(=N3C(=N2)N(C3)C4CCCCC4NS(=O)(=O)C5=CC=C(C=C5)OC(F)(F)F)C6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	698.0 (M + H)	4.59
2450	 <chem>COc1ccc(N2C(=N3C(=N2)N(C3)C4CCCCC4NS(=O)(=O)C5=CC=C(C=C5)OC(F)(F)F)C6=CC=CC=C6)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	694.2 (M + H)	4.42
2451	 <chem>Fc1cccc(N2C(=N3C(=N2)N(C3)C4CCCCC4NS(=O)(=O)C5=CC=C(C=C5)OC(F)(F)F)C6=CC=CC=C6)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	682.2 (M + H)	4.42
2452	 <chem>CN1C(=N2C(=N1)N(C2)C3CCCCC3NS(=O)(=O)C4=CC=C(C=C4)OC(F)(F)F)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	4.28

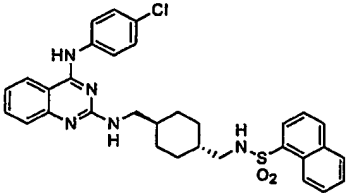
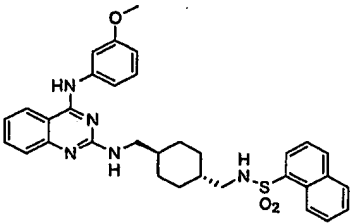
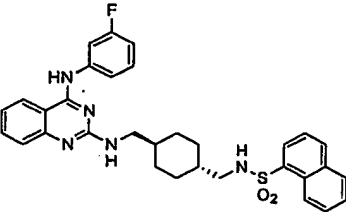
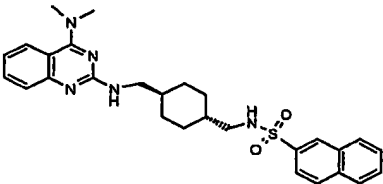
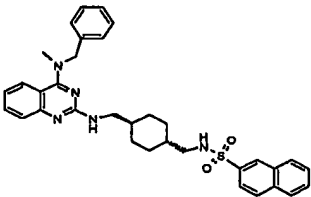
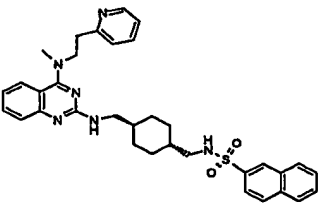
Example No.	Structure	ESI-MS	Retention Time (min)
2453	 $\text{CF}_3\text{CO}_2\text{H}$	666.2 (M + H)	4.61
2454	 $2\text{CF}_3\text{CO}_2\text{H}$	681.2 (M + H)	3.72
2455	 $\text{CF}_3\text{CO}_2\text{H}$	632.4 (M + H)	4.21
2456	 $2\text{CF}_3\text{CO}_2\text{H}$	707.2 (M + H)	4.70
2457	 $\text{CF}_3\text{CO}_2\text{H}$	673.2 (M + H)	3.94
2458	 $\text{CF}_3\text{CO}_2\text{H}$	576.2 (M + H)	4.16

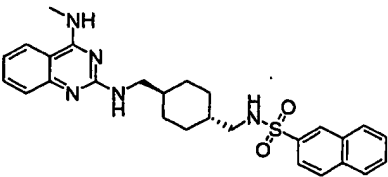
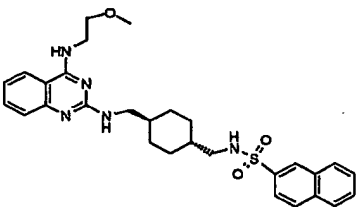
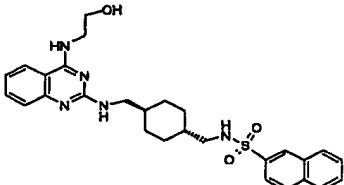
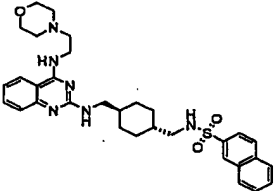
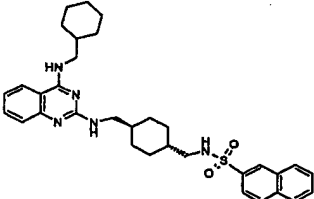
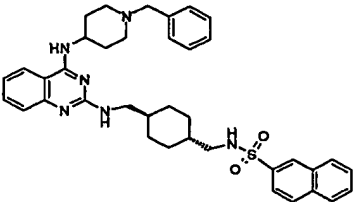
Example No.	Structure	ESI-MS	Retention Time (min)
2459	 $\text{CF}_3\text{CO}_2\text{H}$	620.4 (M + H)	4.19
2460	 $\text{CF}_3\text{CO}_2\text{H}$	606.6 (M + H)	3.94
2461	 $2\text{CF}_3\text{CO}_2\text{H}$	675.4 (M + H)	3.59
2462	 $\text{CF}_3\text{CO}_2\text{H}$	658.6 (M + H)	4.82
2463	 $2\text{CF}_3\text{CO}_2\text{H}$	735.4 (M + H)	3.82
2464	 $\text{CF}_3\text{CO}_2\text{H}$	696.0 (M + H)	4.56

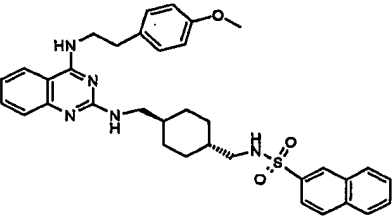
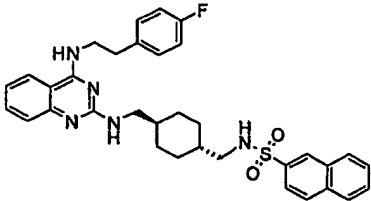
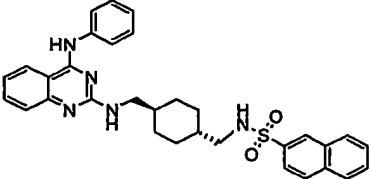
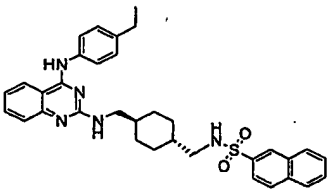
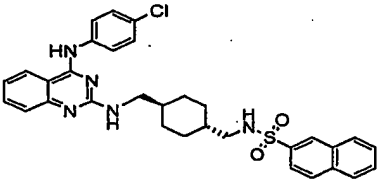
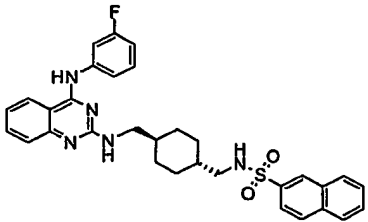
Example No.	Structure	ESI-MS	Retention Time (min)
2465	 <chem>CF3CO2H</chem>	684.4 (M + H)	4.61
2466	 <chem>2CF3CO2H</chem>	670.2 (M + H)	3.56
2467	 <chem>CF3CO2H</chem>	638.2 (M + H)	4.43
2468	 <chem>CF3CO2H</chem>	666.2 (M + H)	4.68
2469	 <chem>CF3CO2H</chem>	672.2 (M + H)	4.60
2470	 <chem>CF3CO2H</chem>	668.2 (M + H)	4.44

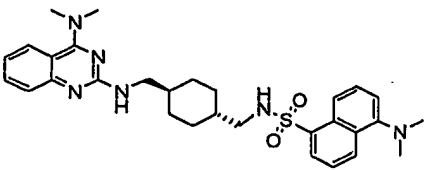
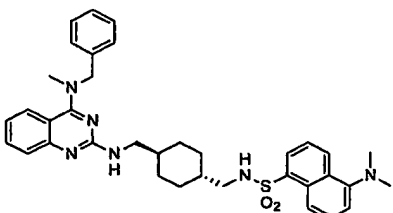
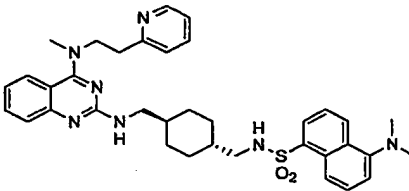
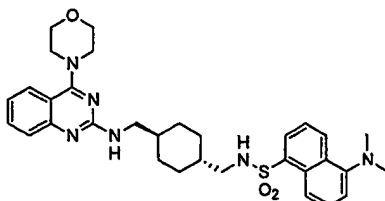
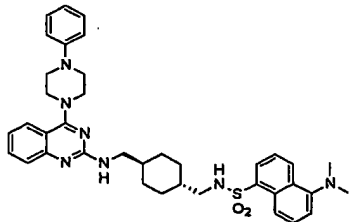
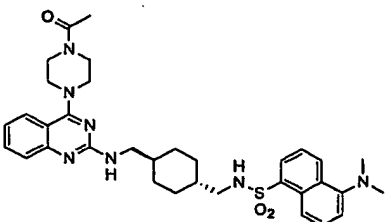
Example No.	Structure	ESI-MS	Retention Time (min)
2471	 <p>CF₃CO₂H</p>	656.4 (M + H)	4.47
2472	 <p>2CF₃CO₂H</p>	595.4 (M + H)	3.32
2473	 <p>CF₃CO₂H</p>	534.0 (M + H)	3.81
2474	 <p>CF₃CO₂H</p>	520.4 (M + H)	3.56
2475	 <p>2CF₃CO₂H</p>	589.2 (M + H)	3.25
2476	 <p>CF₃CO₂H</p>	572.4 (M + H)	4.47

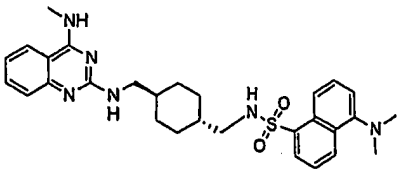
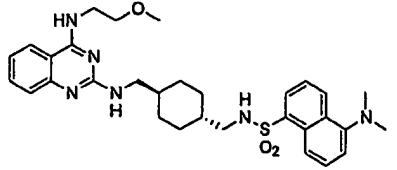
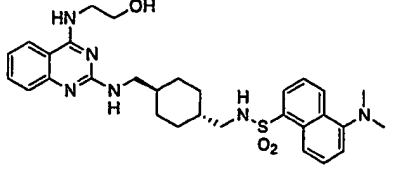
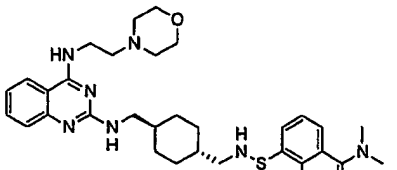
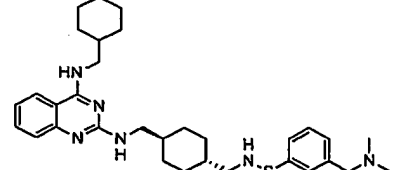
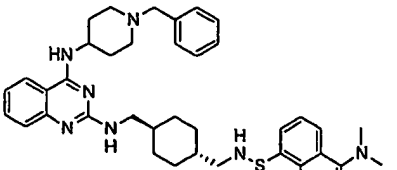
Example No.	Structure	ESI-MS	Retention Time (min)
2477	 2CF ₃ CO ₂ H	649.4 (M + H)	3.50
2478	 CF ₃ CO ₂ H	610.4 (M + H)	4.26
2479	 CF ₃ CO ₂ H	598.2 (M + H)	4.30
2480	 2CF ₃ CO ₂ H	584.4 (M + H)	3.29
2481	 CF ₃ CO ₂ H	552.6 (M + H)	4.11
2482	 CF ₃ CO ₂ H	580.6 (M + H)	4.40

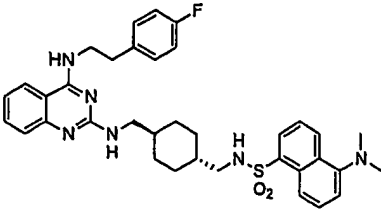
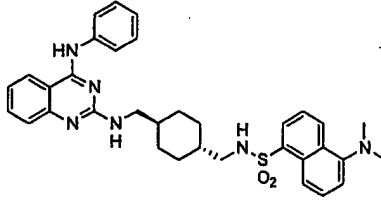
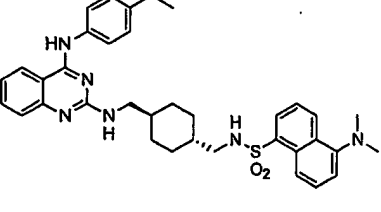
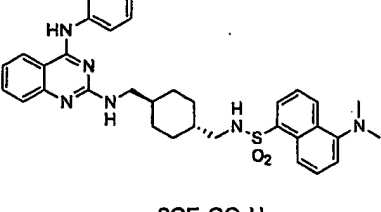
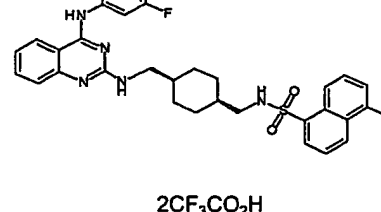
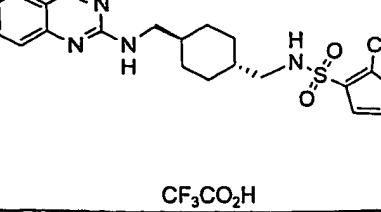
Example No.	Structure	ESI-MS	Retention Time (min)
2483	 <chem>Clc1ccc(Nc2nc3ccccc3n2C4CCCCC4NS(=O)(=O)c5ccc6ccccc65)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	4.30
2484	 <chem>COc1ccc(Nc2nc3ccccc3n2C4CCCCC4NS(=O)(=O)c5ccc6ccccc65)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	582.4 (M + H)	4.14
2485	 <chem>Fc1ccc(Nc2nc3ccccc3n2C4CCCCC4NS(=O)(=O)c5ccc6ccccc65)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	4.14
2486	 <chem>CN1C=NC2=C(N1)C(=NC=C2C3CCCCC3NS(=O)(=O)c4ccc5ccccc54)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.94
2487	 <chem>CN1C=NC2=C(N1)C(=NC=C2C3CCCCC3NS(=O)(=O)c4ccc5ccccc54)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.6 (M + H)	4.34
2488	 <chem>CN1C=NC2=C(N1)C(=NC=C2C3CCCCC3NS(=O)(=O)c4ccc5ccccc54)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	595.2 (M + H)	3.41

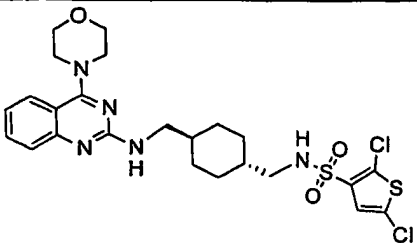
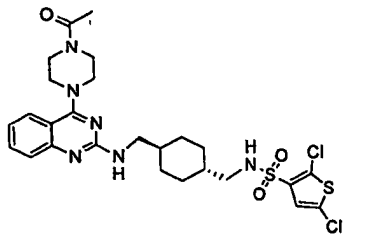
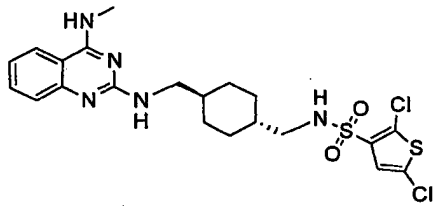
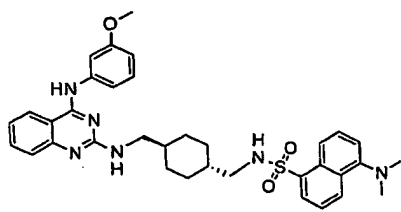
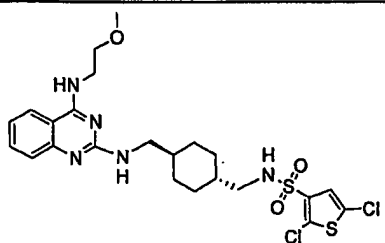
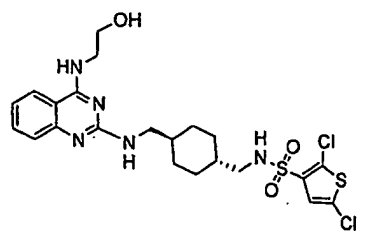
Example No.	Structure	ESI-MS	Retention Time (min)
2489	 <chem>CCNc1nc2ccccc2n1C[C@H]3CCCC[C@H]3CS(=O)(=O)c4ccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.84
2490	 <chem>COCCNc1nc2ccccc2n1C[C@H]3CCCC[C@H]3CS(=O)(=O)c4ccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.2 (M + H)	3.84
2491	 <chem>OCCNc1nc2ccccc2n1C[C@H]3CCCC[C@H]3CS(=O)(=O)c4ccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	520.4 (M + H)	3.60
2492	 <chem>C1CCN(C1)CCNC2=NC3=CC=CC=C3N=C2C[C@H]4CCCC[C@H]4CS(=O)(=O)c5ccc6ccccc56</chem> $2\text{CF}_3\text{CO}_2\text{H}$	589.2 (M + H)	3.29
2493	 <chem>C1CCCCC1CNc2nc3ccccc3n2C[C@H]4CCCC[C@H]4CS(=O)(=O)c5ccc6ccccc56</chem> $\text{CF}_3\text{CO}_2\text{H}$	572.4 (M + H)	4.51
2494	 <chem>c1ccc(cc1)CN2CCCCC2Nc3nc4ccccc4n3C[C@H]5CCCC[C@H]5CS(=O)(=O)c6ccc7ccccc67</chem> $2\text{CF}_3\text{CO}_2\text{H}$	649.4 (M + H)	3.52

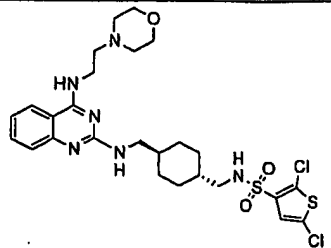
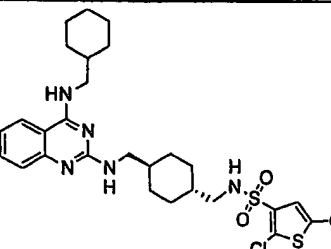
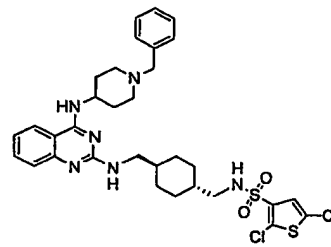
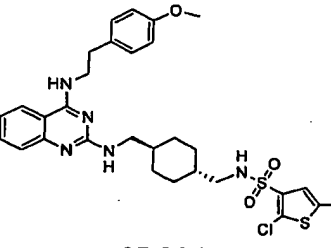
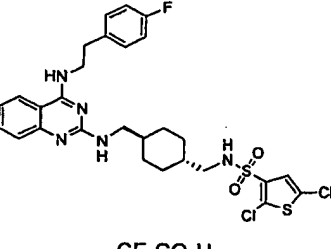
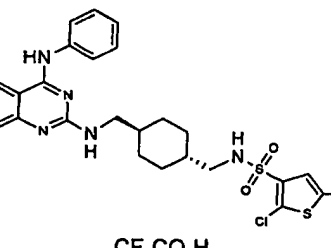
Example No.	Structure	ESI-MS	Retention Time (min)
2495	 <chem>COc1ccc(cc1)CNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	610.2 (M + H)	4.29
2496	 <chem>Fc1ccc(cc1)CNc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	4.34
2497	 <chem>c1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	4.13
2498	 <chem>CCc1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.6 (M + H)	4.37
2499	 <chem>Clc1ccc(cc1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	4.30
2500	 <chem>Fc1cccc(c1)Nc2nc3ccccc3n2CNC4CCCCC4NS(=O)(=O)c5ccc6ccccc65</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	4.18

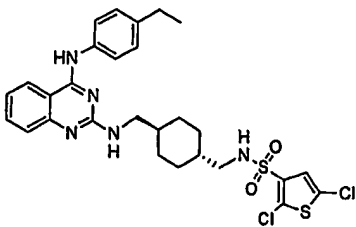
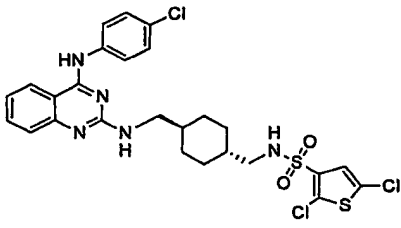
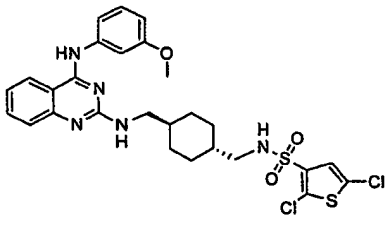
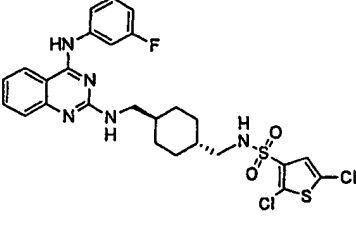
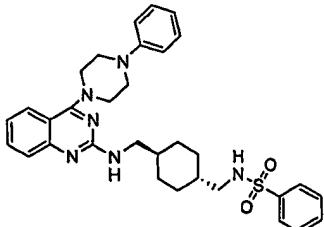
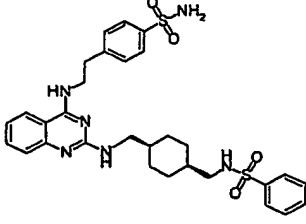
Example No.	Structure	ESI-MS	Retention Time (min)
2501	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	547.4 (M + H)	3.69
2502	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	4.10
2503	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $3\text{CF}_3\text{CO}_2\text{H}$	638.2 (M + H)	3.20
2504	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	589.2 (M + H)	3.62
2505	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $3\text{CF}_3\text{CO}_2\text{H}$	664.4 (M + H)	4.25
2506	 <chem>CN(C)Cc1nc2c(ncn2C1CCN(C)C1)nc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	3.35

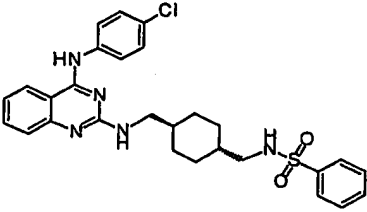
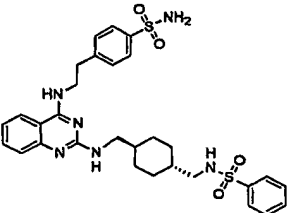
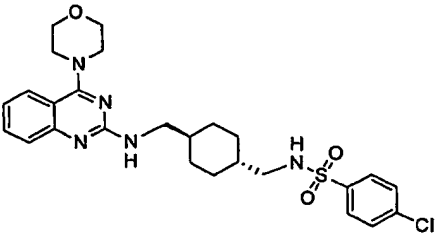
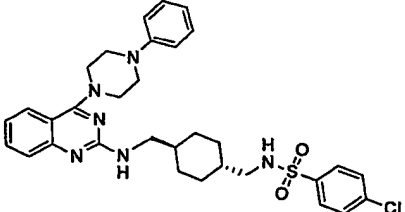
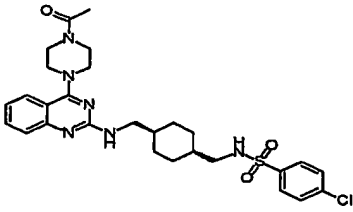
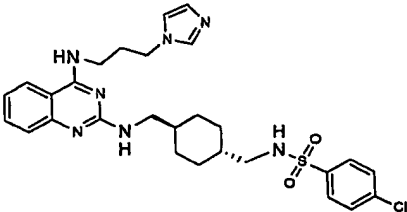
Example No.	Structure	ESI-MS	Retention Time (min)
2507	 $2\text{CF}_3\text{CO}_2\text{H}$	533.2 (M + H)	3.57
2508	 $2\text{CF}_3\text{CO}_2\text{H}$	577.6 (M + H)	3.58
2509	 $2\text{CF}_3\text{CO}_2\text{H}$	563.2 (M + H)	3.28
2510	 $3\text{CF}_3\text{CO}_2\text{H}$	632.6 (M + H)	3.06
2511	 $2\text{CF}_3\text{CO}_2\text{H}$	615.4 (M + H)	4.30
2512	 $3\text{CF}_3\text{CO}_2\text{H}$	692.2 (M + H)	3.38

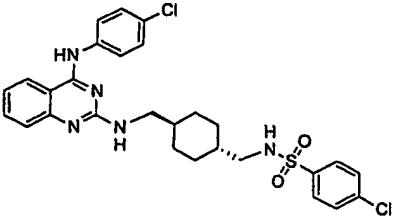
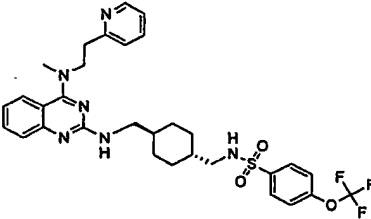
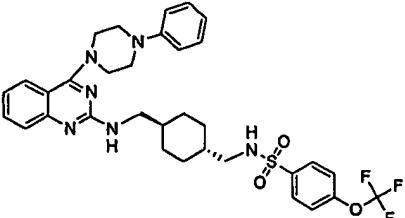
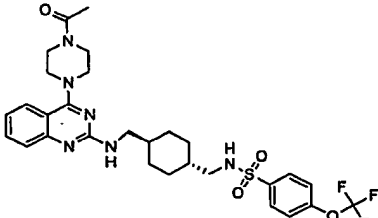
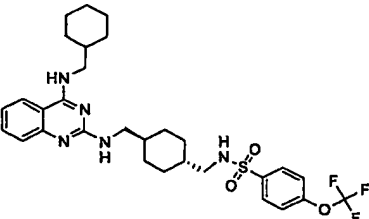
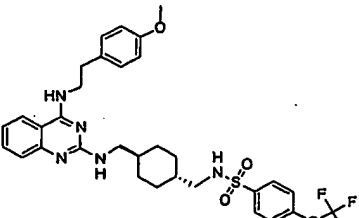
Example No.	Structure	ESI-MS	Retention Time (min)
2513	 <chem>2CF3CO2H</chem>	641.4 (M + H)	4.13
2514	 <chem>2CF3CO2H</chem>	595.4 (M + H)	3.89
2515	 <chem>2CF3CO2H</chem>	623.4 (M + H)	4.20
2516	 <chem>2CF3CO2H</chem>	629.2 (M + H)	4.15
2517	 <chem>2CF3CO2H</chem>	613.2 (M + H)	4.02
2518	 <chem>CF3CO2H</chem>	528.2 (M + H)	4.03

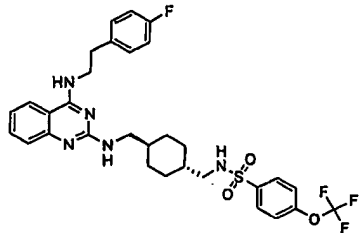
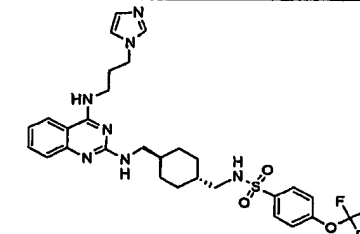
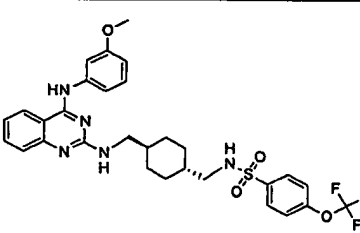
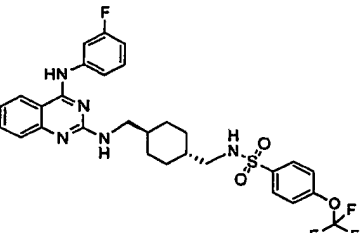
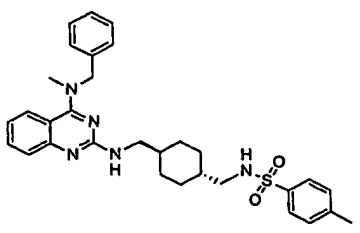
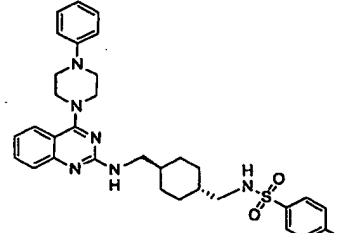
Example No.	Structure	ESI-MS	Retention Time (min)
2519	 <chem>CC1(C)CCCC1CNc2nc3ccccc3n2N[C@@H](C1CCCCC1)S(=O)(=O)c2cc(Cl)cc(Cl)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	3.96
2520	 <chem>CC(=O)N1CCN(CC1)Nc2nc3ccccc3n2N[C@@H](C1CCCCC1)S(=O)(=O)c2cc(Cl)cc(Cl)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	611.0 (M + H)	3.69
2521	 <chem>CNc1nc2ccccc2n1N[C@@H](C1CCCCC1)S(=O)(=O)c2cc(Cl)cc(Cl)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.2 (M + H)	3.94
2522	 <chem>COc1ccc(Nc2nc3ccccc3n2N[C@@H](C1CCCCC1)S(=O)(=O)c2c(C)ccc3[nH]c4ccccc43)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	625.4 (M + H)	3.94
2523	 <chem>COCCNc1nc2ccccc2n1N[C@@H](C1CCCCC1)S(=O)(=O)c2cc(Cl)cc(Cl)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	558.2 (M + H)	3.96
2524	 <chem>OCCNc1nc2ccccc2n1N[C@@H](C1CCCCC1)S(=O)(=O)c2cc(Cl)cc(Cl)c2</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.2 (M + H)	3.67

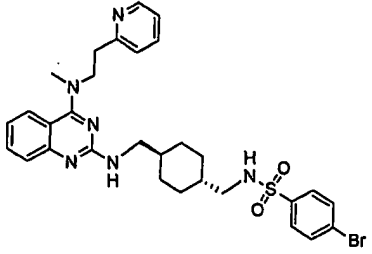
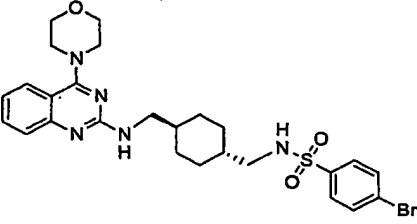
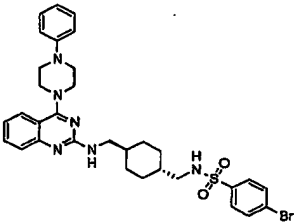
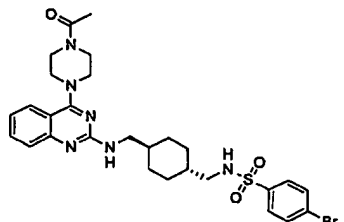
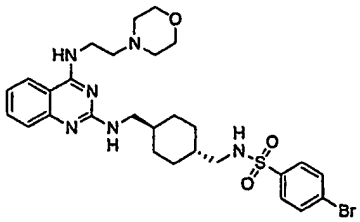
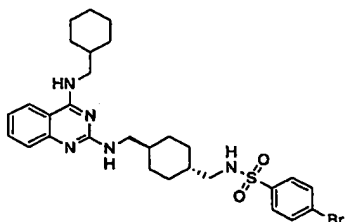
Example No.	Structure	ESI-MS	Retention Time (min)
2525	 $2\text{CF}_3\text{CO}_2\text{H}$	613.2 (M + H)	3.31
2526	 $\text{CF}_3\text{CO}_2\text{H}$	596.2 (M + H)	4.69
2527	 $2\text{CF}_3\text{CO}_2\text{H}$	673.4 (M + H)	3.57
2528	 $\text{CF}_3\text{CO}_2\text{H}$	634.4 (M + H)	4.41
2529	 $\text{CF}_3\text{CO}_2\text{H}$	622.2 (M + H)	4.45
2530	 $\text{CF}_3\text{CO}_2\text{H}$	576 (M + H)	4.25

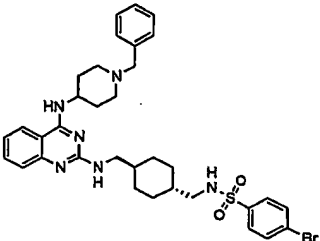
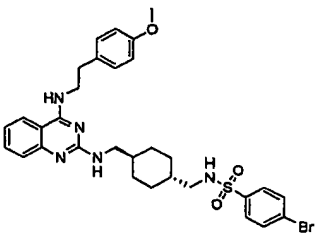
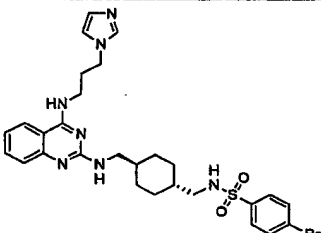
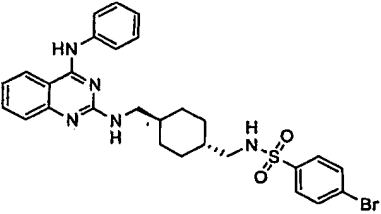
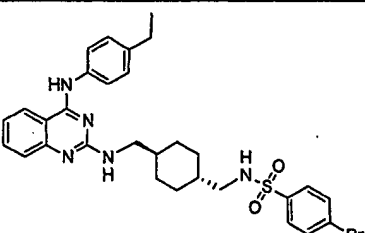
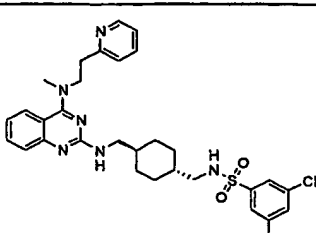
Example No.	Structure	ESI-MS	Retention Time (min)
2531	 $\text{CF}_3\text{CO}_2\text{H}$	604.4 (M + H)	4.52
2532	 $\text{CF}_3\text{CO}_2\text{H}$	610.2 (M + H)	4.40
2533	 $\text{CF}_3\text{CO}_2\text{H}$	606.4 (M + H)	4.29
2534	 $\text{CF}_3\text{CO}_2\text{H}$	594.2 (M + H)	4.27
2535	 $2\text{CF}_3\text{CO}_2\text{H}$	571.8 (M + H)	4.99
2536	 $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.43

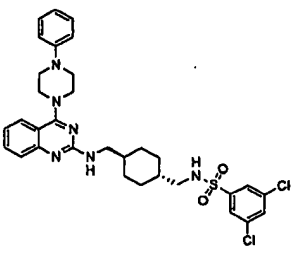
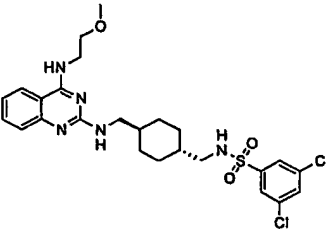
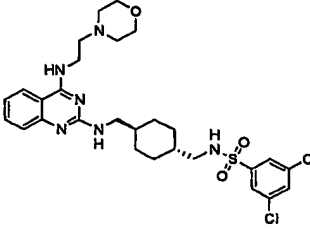
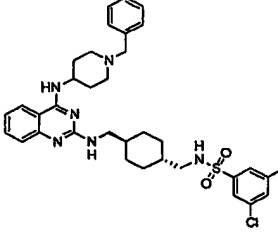
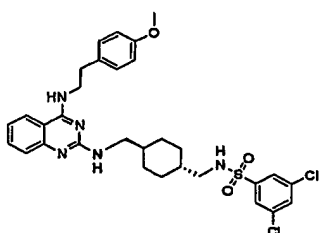
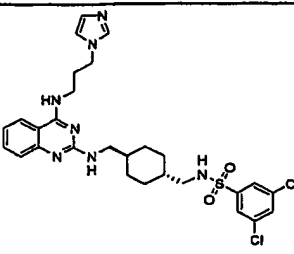
Example No.	Structure	ESI-MS	Retention Time (min)
2537	 <chem>Clc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4CS(=O)(=O)c5ccccc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	4.86
2538	 <chem>NC(=O)S(=O)c1ccc(NC2=NC3=CC=CC=C3N2CNC4CCCCC4CS(=O)(=O)c5ccccc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	5.13
2539	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5COCCO5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.6 (M + H)	4.65
2540	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5CN(CCN5c6ccccc6)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	605.6 (M + H)	5.21
2541	 <chem>CC(=O)N1CCN(C1C2=NC3=CC=CC=C3N2CNC4CCCCC4CS(=O)(=O)c5ccccc5Cl)CC6=CC=CC=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.45
2542	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5=NC=CC=C5)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	568.8 (M + H)	4.09

Example No.	Structure	ESI-MS	Retention Time (min)
2543	 <chem>Clc1ccc(Nc2nc3ccccc3n2C[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(Cl)cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.11
2544	 <chem>CN(C)Cc1cccnc1C2=NC3=CC=CC=C3N=C2C[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	629.6 (M + H)	4.37
2545	 <chem>c1ccc(cc1)N2CCN(CC2)Cc3nc4ccccc4n3C[C@H]5CCCC[C@H]5NS(=O)(=O)c6ccc(OC(F)(F)F)cc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	655.6 (M + H)	5.35
2546	 <chem>CC(=O)N1CCN(CC1)Cc2nc3ccccc3n2C[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	621.8 (M + H)	4.63
2547	 <chem>C1CCCCC1Cc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	606.8 (M + H)	5.45
2548	 <chem>COc1ccc(cc1)Cc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.6 (M + H)	5.21

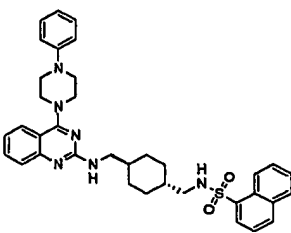
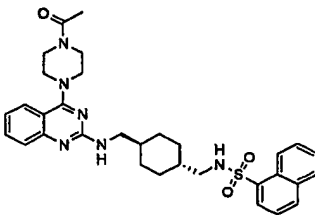
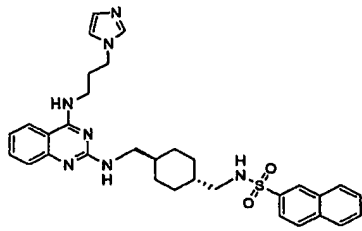
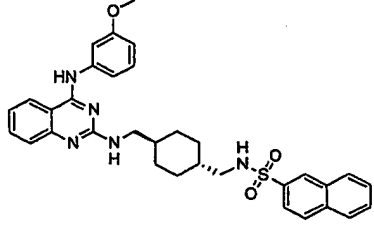
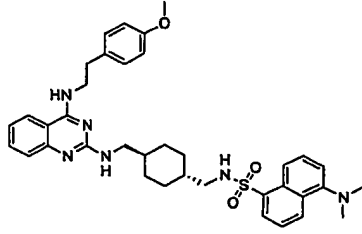
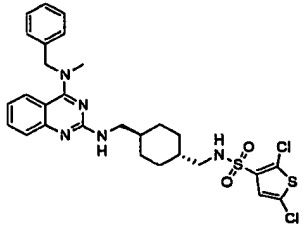
Example No.	Structure	ESI-MS	Retention Time (min)
2549	 $\text{CF}_3\text{CO}_2\text{H}$	632.6 (M + H)	5.25
2550	 $2\text{CF}_3\text{CO}_2\text{H}$	618.6 (M + H)	4.29
2551	 $\text{CF}_3\text{CO}_2\text{H}$	616.6 (M + H)	5.14
2552	 $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	5.13
2553	 $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	5.03
2554	 $2\text{CF}_3\text{CO}_2\text{H}$	585.6 (M + H)	5.13

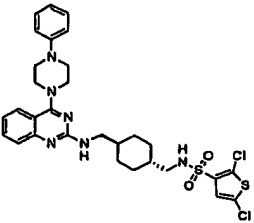
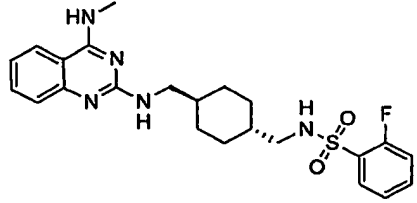
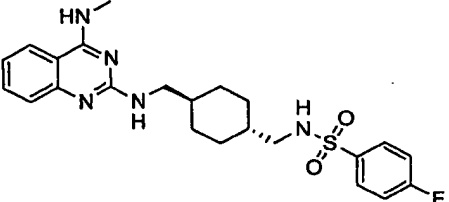
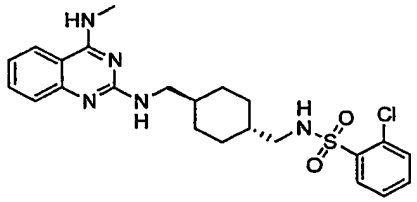
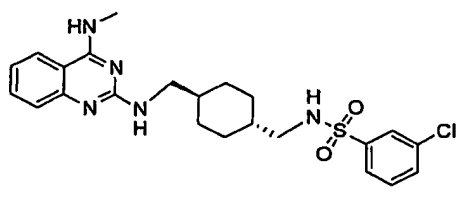
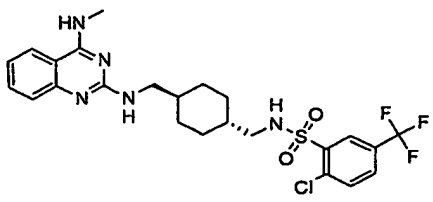
Example No.	Structure	ESI-MS	Retention Time (min)
2555	 2CF ₃ CO ₂ H	623.6 (M + H)	4.25
2556	 CF ₃ CO ₂ H	574.6 (M + H)	4.73
2557	 2CF ₃ CO ₂ H	649.0 (M + H)	5.25
2558	 CF ₃ CO ₂ H	615.0 (M + H)	4.51
2559	 2CF ₃ CO ₂ H	617.4 (M + H)	4.15
2560	 CF ₃ CO ₂ H	600.6 (M + H)	5.37

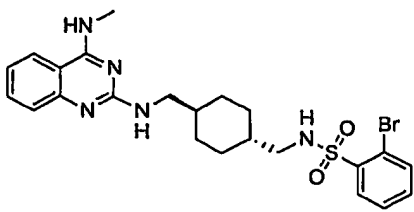
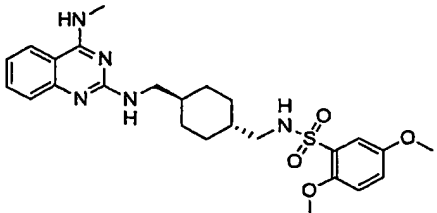
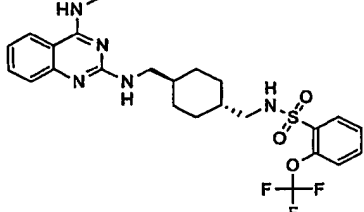
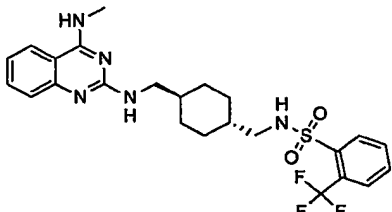
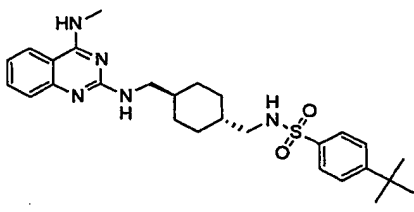
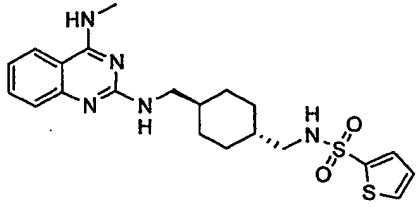
Example No.	Structure	ESI-MS	Retention Time (min)
2561	 2CF ₃ CO ₂ H	677.0 (M + H)	4.45
2562	 CF ₃ CO ₂ H	638.6 (M + H)	5.18
2563	 2CF ₃ CO ₂ H	612.6 (M + H)	4.16
2564	 CF ₃ CO ₂ H	580.0 (M + H)	5.01
2565	 CF ₃ CO ₂ H	608.0 (M + H)	5.26
2566	 2CF ₃ CO ₂ H	613.6 (M + H)	4.44

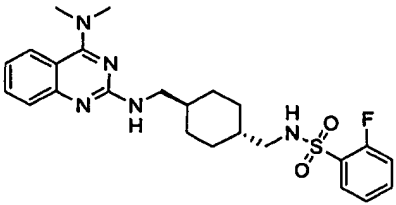
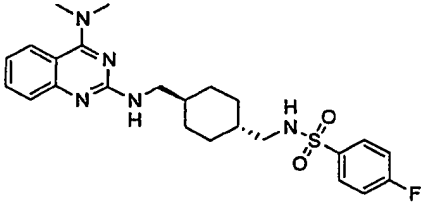
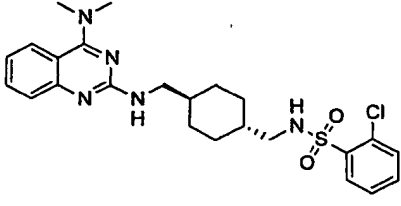
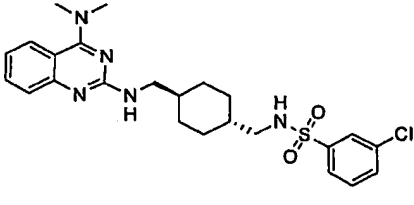
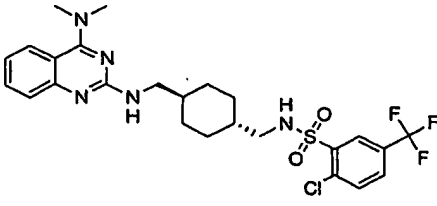
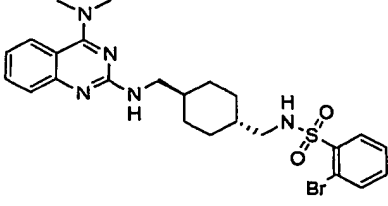
Example No.	Structure	ESI-MS	Retention Time (min)
2567	 2CF ₃ CO ₂ H	639.6 (M + H)	5.48
2568	 CF ₃ CO ₂ H	552.6 (M + H)	4.92
2569	 2CF ₃ CO ₂ H	607.8 (M + H)	4.33
2570	 2CF ₃ CO ₂ H	667.4 (M + H)	4.67
2571	 CF ₃ CO ₂ H	628.6 (M + H)	5.29
2572	 2CF ₃ CO ₂ H	602.6 (M + H)	4.35

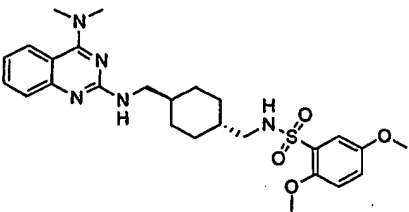
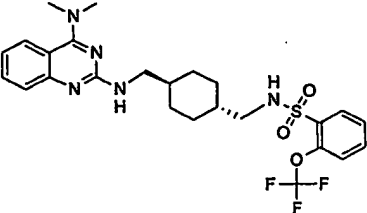
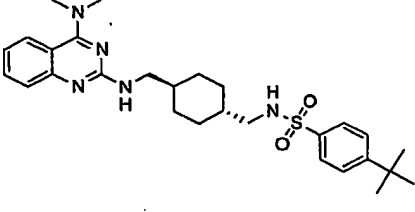
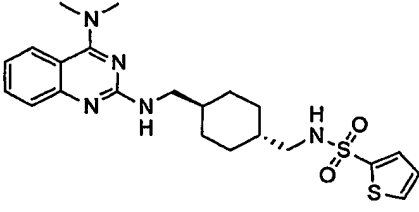
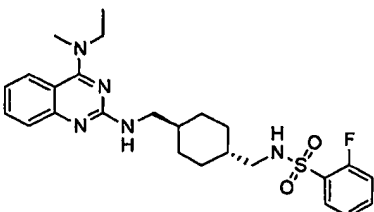
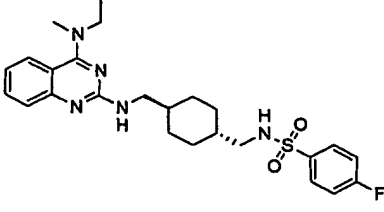
Example No.	Structure	ESI-MS	Retention Time (min)
2573	 <chem>Clc1ccc(cc1)S(=O)(=O)N[C@@H]2CCCC[C@H]2CNc3nc4ccccc4n3Nc5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.23
2574	 <chem>FC(F)(F)Oc1ccc(cc1)S(=O)(=O)N[C@@H]2CCCC[C@H]2CNc3nc4ccccc4n3NCCc5ccc(cc5)S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	805.4 (M + H)	4.91
2575	 <chem>FC(F)(F)Oc1ccc(cc1)S(=O)(=O)N[C@@H]2CCCC[C@H]2CNc3nc4ccccc4n3NCCc5c[nH]n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	730.8 (M + H)	4.47
2576	 <chem>Brc1ccc(cc1)Oc2ccc(cc2)S(=O)(=O)N[C@@H]3CCCC[C@H]3CNc4nc5ccccc5n4NCCc6ccc(cc6)S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	771.6 (M + H)	4.93
2577	 <chem>FC(F)(F)c1ccc(cc1)Oc2ccc(cc2)S(=O)(=O)N[C@@H]3CCCC[C@H]3CNc4nc5ccccc5n4NCCc6ccc(cc6)S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	745.6 (M + H)	5.01
2578	 <chem>c1ccc2cc3c(c1)nc4ccccc4n3C[C@H]5CCCC[C@H]5CNc6c7ccccc7c8ccccc68S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.8 (M + H)	5.18

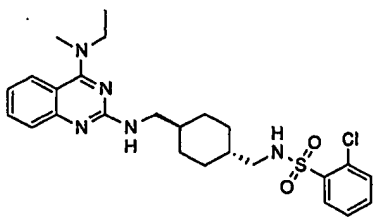
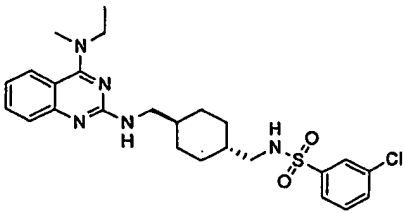
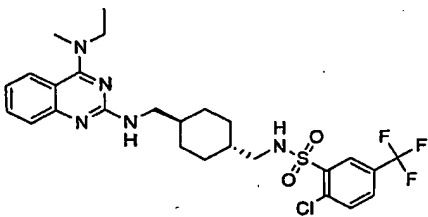
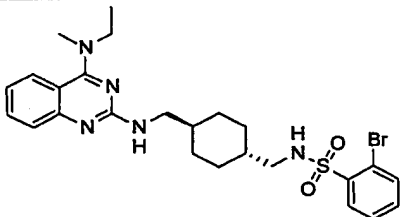
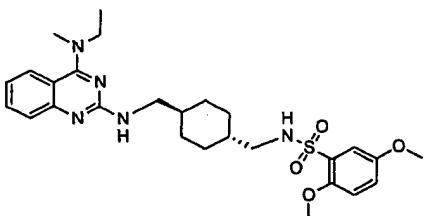
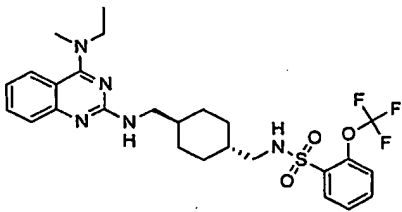
Example No.	Structure	ESI-MS	Retention Time (min)
2579	 <p>2CF₃CO₂H</p>	621.8 (M + H)	5.27
2580	 <p>CF₃CO₂H</p>	587.6 (M + H)	4.51
2581	 <p>2CF₃CO₂H</p>	584.6 (M + H)	4.21
2582	 <p>CF₃CO₂H</p>	582.8 (M + H)	5.03
2583	 <p>CF₃CO₂H</p>	653.8 (M + H)	4.90
2584	 <p>CF₃CO₂H</p>	604.6 (M + H)	5.33

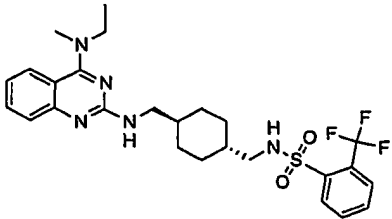
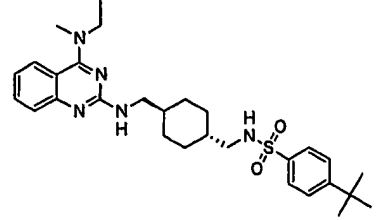
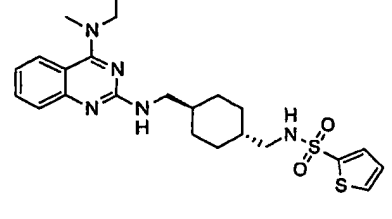
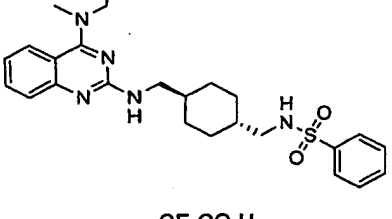
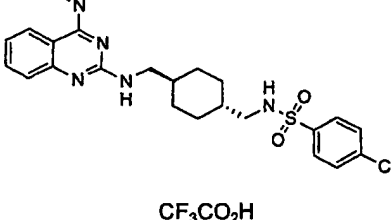
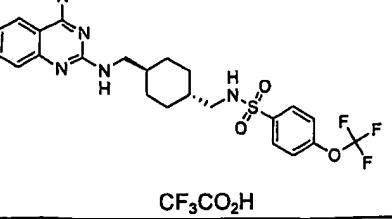
Example No.	Structure	ESI-MS	Retention Time (min)
2585	 $2\text{CF}_3\text{CO}_2\text{H}$	645.6 (M + H)	5.41
2586	 $\text{CF}_3\text{CO}_2\text{H}$	458.6 (M + H)	4.39
2587	 $\text{CF}_3\text{CO}_2\text{H}$	458.6 (M + H)	4.40
2588	 $\text{CF}_3\text{CO}_2\text{H}$	474.6 (M + H)	4.39
2589	 $\text{CF}_3\text{CO}_2\text{H}$	474.6 (M + H)	4.58
2590	 $\text{CF}_3\text{CO}_2\text{H}$	542.6 (M + H)	4.79

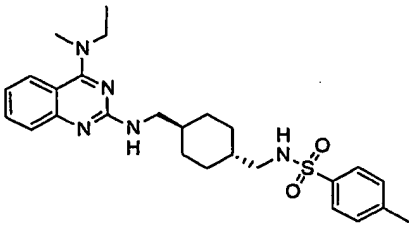
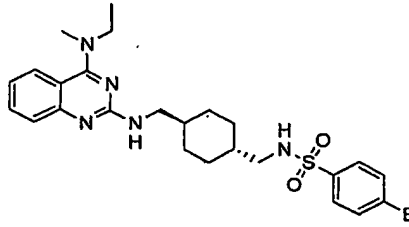
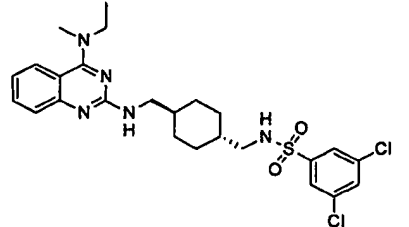
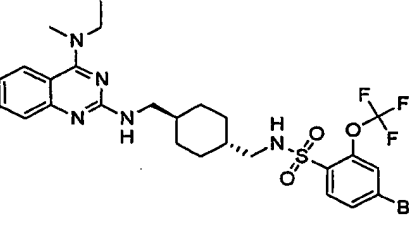
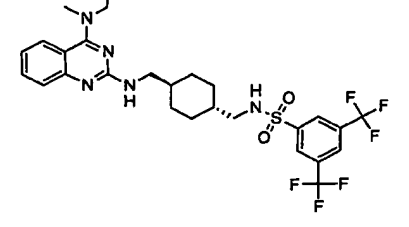
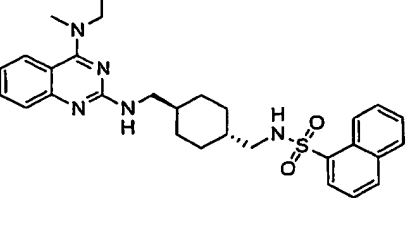
Example No.	Structure	ESI-MS	Retention Time (min)
2591	 <chem>CC1=NC2=C(N1)N=CN=C2NCC3CCCCC3NS(=O)(=O)c4cc(Br)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.51
2592	 <chem>COc1cc(OC)cc(S(=O)(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.33
2593	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	4.61
2594	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)NCC2CCCCC2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.6 (M + H)	4.57
2595	 <chem>CC(C)(C)c1ccc(S(=O)(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.87
2596	 <chem>Cc1nc2ccccc2n1NCC3CCCCC3NS(=O)(=O)c4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.8 (M + H)	4.29

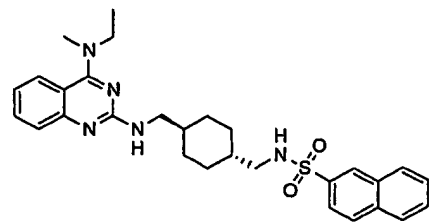
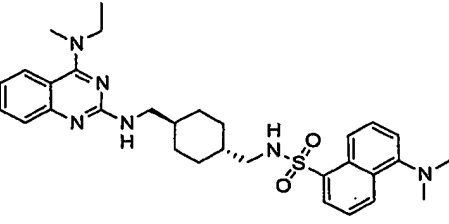
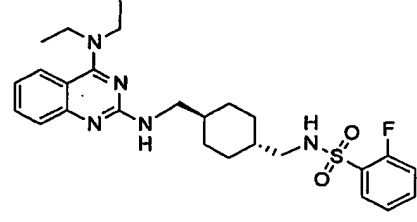
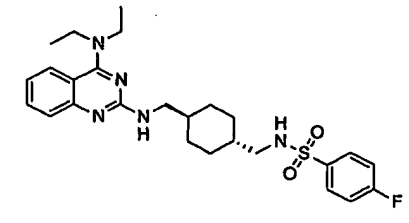
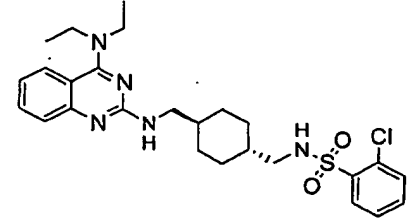
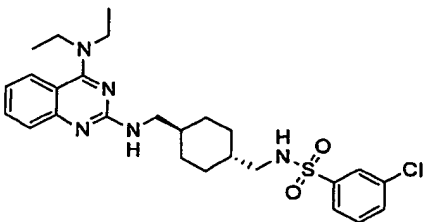
Example No.	Structure	ESI-MS	Retention Time (min)
2597	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4ccccc4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.47
2598	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.53
2599	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4ccccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.55
2600	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4ccccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	487.6 (M + H)	4.65
2601	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4cc(Cl)ccc4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.6 (M + H)	4.91
2602	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3NS(=O)(=O)c4ccccc4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	4.61

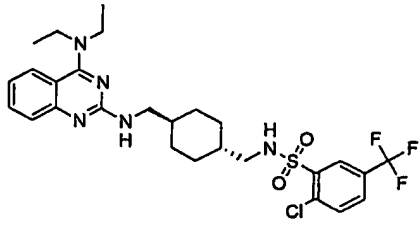
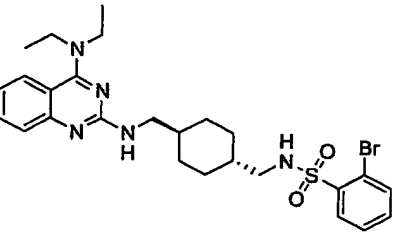
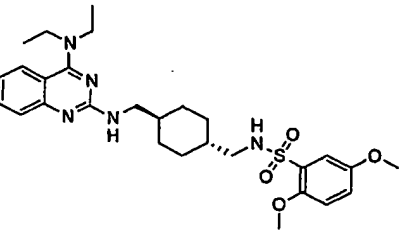
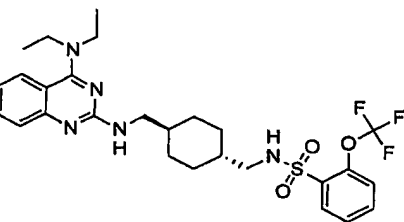
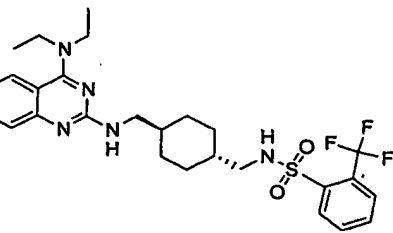
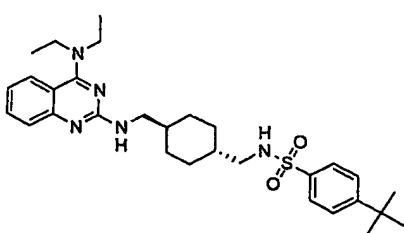
Example No.	Structure	ESI-MS	Retention Time (min)
2603	 <chem>COc1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.8 (M + H)	4.43
2604	 <chem>FC(F)(F)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.6 (M + H)	4.80
2605	 <chem>CC(C)(C)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.6 (M + H)	5.00
2606	 <chem>c1cc(S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3)sc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.6 (M + H)	4.40
2607	 <chem>Fc1ccccc1S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.60
2608	 <chem>Fc1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.6 (M + H)	4.64

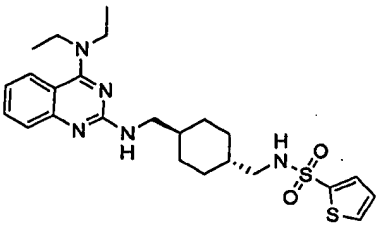
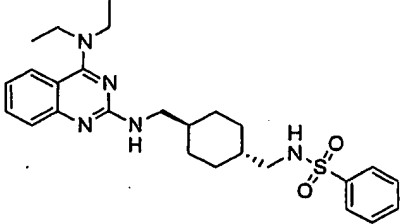
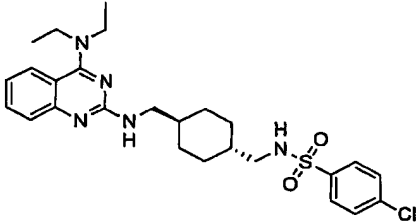
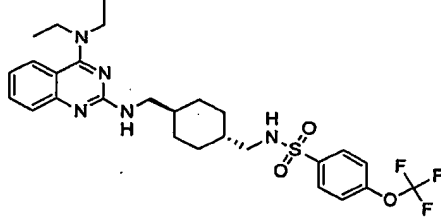
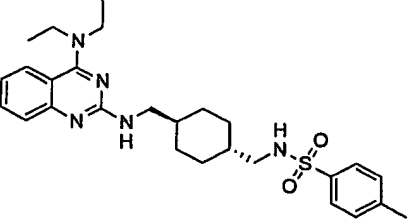
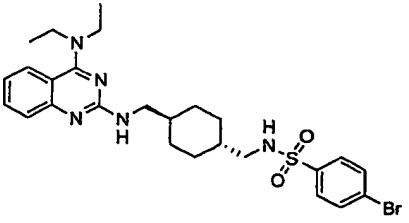
Example No.	Structure	ESI-MS	Retention Time (min)
2609	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)C3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	4.74
2610	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cccc(Cl)c4)C3CCCCC3NS(=O)(=O)c4cccc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.86
2611	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)ccc4Cl)C3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)ccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.8 (M + H)	5.00
2612	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cccc(Br)c4)C3CCCCC3NS(=O)(=O)c4cccc(Br)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.0 (M + H)	4.80
2613	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(OC)cc(OC)c4)C3CCCCC3NS(=O)(=O)c4cc(OC)cc(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.63
2614	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(OC(F)(F)F)ccc4)C3CCCCC3NS(=O)(=O)c4cc(OC(F)(F)F)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.90

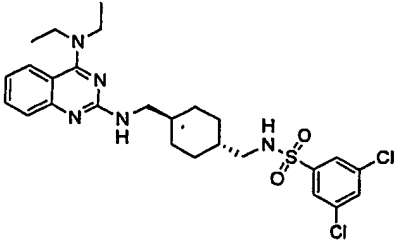
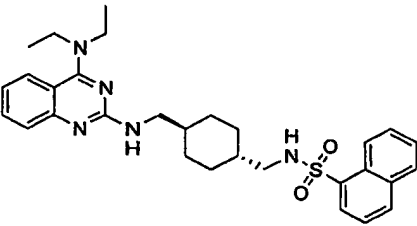
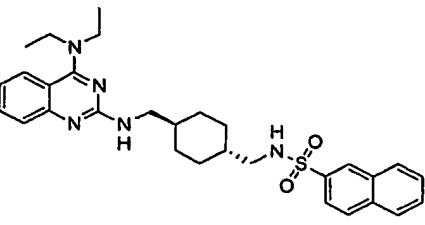
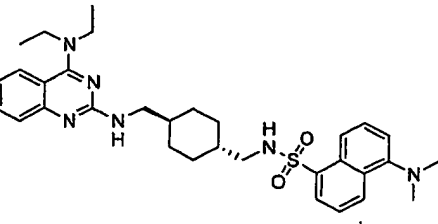
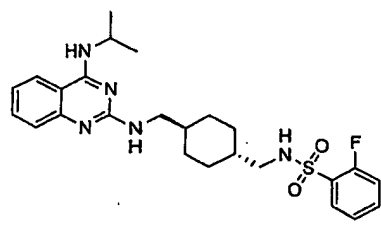
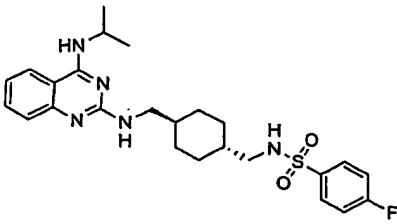
Example No.	Structure	ESI-MS	Retention Time (min)
2615	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccccc3C(F)(F)F)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	4.82
2616	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccc(C(C)(C)C)cc3)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.8 (M + H)	5.07
2617	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccsc3)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.6 (M + H)	4.55
2618	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccccc3)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	4.59
2619	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccc(Cl)cc3)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.81
2620	 <chem>CCN(C)c1nc2c(ncn2C1CCN(CS(=O)(=O)c3ccc(OC(F)(F)F)cc3)c3ccccc3)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.94

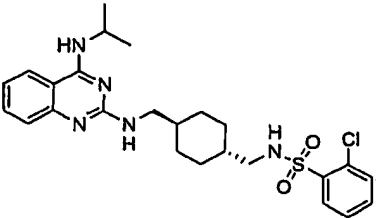
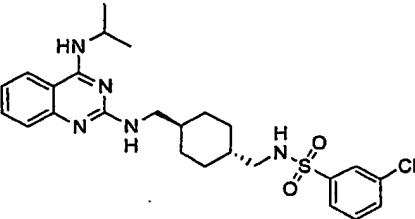
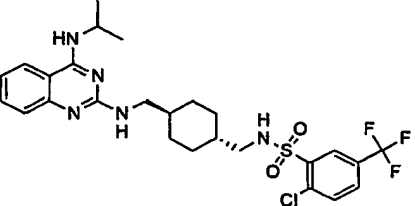
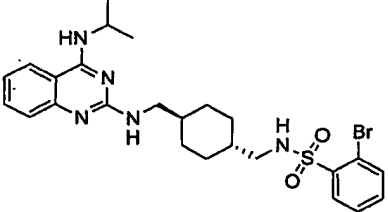
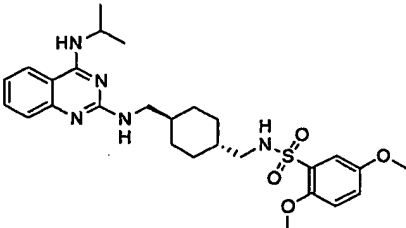
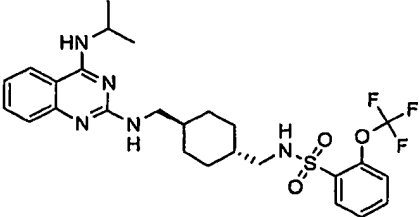
Example No.	Structure	ESI-MS	Retention Time (min)
2621	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(C)cc4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.6 (M + H)	4.73
2622	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(Br)cc4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.85
2623	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(Cl)ccc4Cl)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	5.08
2624	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(OC(F)(F)F)ccc4Br)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	5.11
2625	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)ccc4C(F)(F)F)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	5.16
2626	 <chem>CCN(C)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4c5ccccc5cc4)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.75

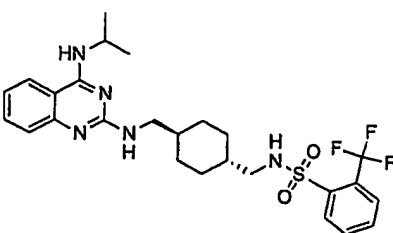
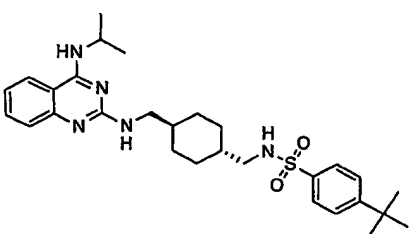
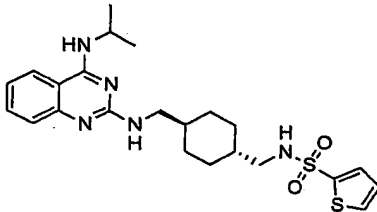
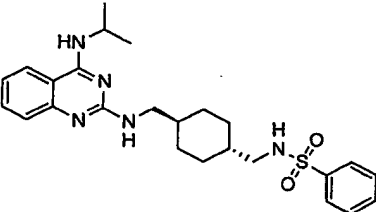
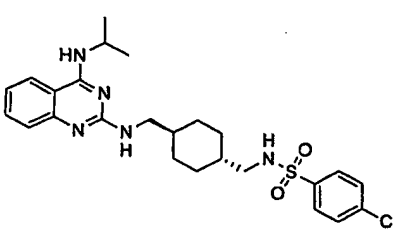
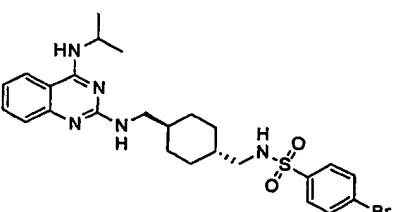
Example No.	Structure	ESI-MS	Retention Time (min)
2627	 <chem>CCN(CC)c1nc2c(ncn2C1CCN3CCCCC3S(=O)(=O)c4ccc5ccccc45)c3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.91
2628	 $2\text{CF}_3\text{CO}_2\text{H}$	561.6 (M + H)	4.61
2629	 $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.75
2630	 $\text{CF}_3\text{CO}_2\text{H}$	500.2 (M + H)	4.85
2631	 $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.81
2632	 $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.95

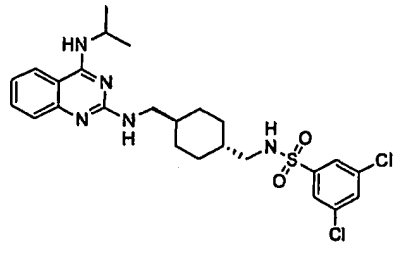
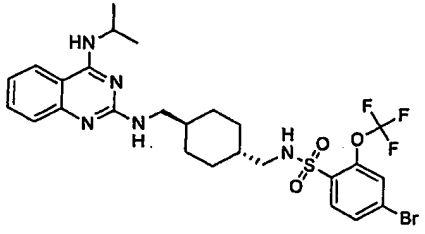
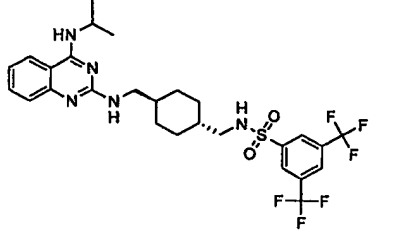
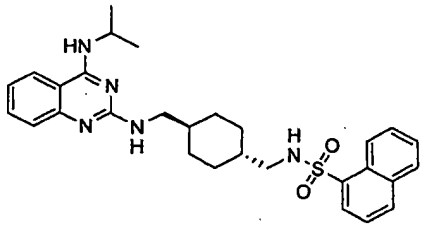
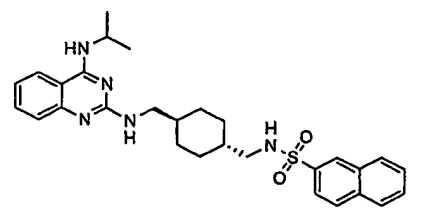
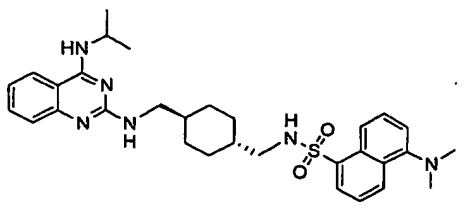
Example No.	Structure	ESI-MS	Retention Time (min)
2633	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(C(F)(F)F)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	584.6 (M + H)	5.18
2634	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccccc4Br)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.6 (M + H)	4.87
2635	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(OC)cc(OC)c4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	542.8 (M + H)	4.80
2636	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(OC(F)(F)F)ccc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.01
2637	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)ccc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.95
2638	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.6 (M + H)	5.20

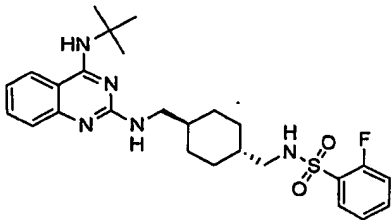
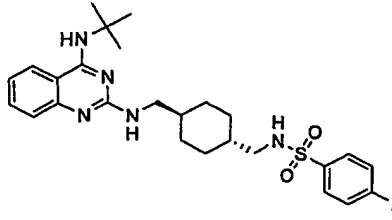
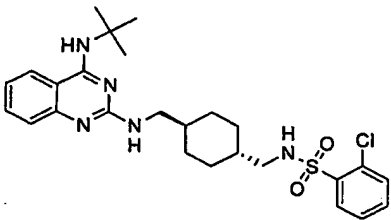
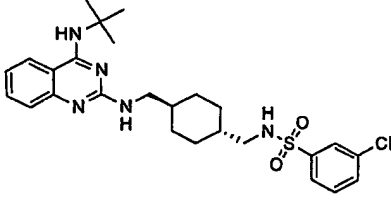
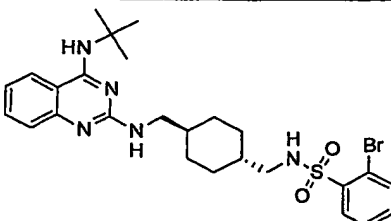
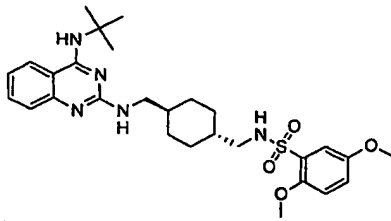
Example No.	Structure	ESI-MS	Retention Time (min)
2639	 CF ₃ CO ₂ H	488.6 (M + H)	4.65
2640	 CF ₃ CO ₂ H	482.6 (M + H)	4.73
2641	 CF ₃ CO ₂ H	516.8 (M + H)	4.97
2642	 CF ₃ CO ₂ H	566.6 (M + H)	5.12
2643	 CF ₃ CO ₂ H	496.8 (M + H)	4.89
2644	 CF ₃ CO ₂ H	560.0 (M + H)	4.98

Example No.	Structure	ESI-MS	Retention Time (min)
2645	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(Cl)ccc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	5.21
2646	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4c5ccccc45)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	4.99
2647	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4c5ccccc45)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.03
2648	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4c5ccccc45N(C)C)cc5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	575.8 (M + H)	4.80
2649	 <chem>CC(C)Nc1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(F)ccc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.64
2650	 <chem>CC(C)Nc1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(F)cc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.66

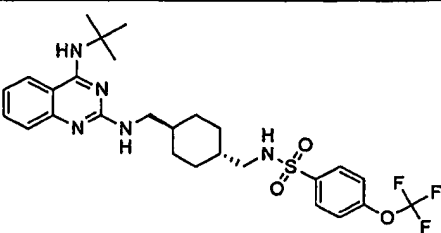
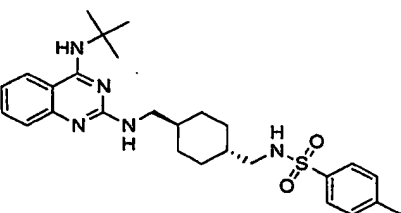
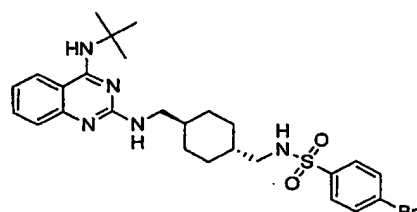
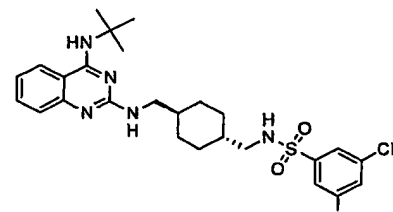
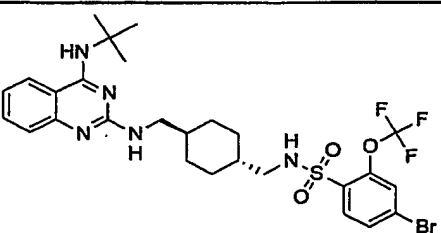
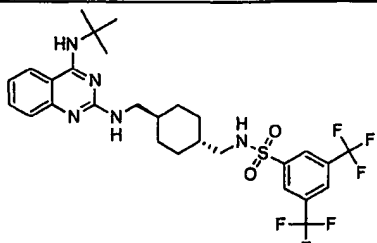
Example No.	Structure	ESI-MS	Retention Time (min)
2651	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3ccccc3Cl)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.72
2652	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cccc(Cl)c3)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.87
2653	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(C(F)(F)F)ccc(Cl)c3)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.03
2654	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3ccccc3Br)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.77
2655	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(OC)cc(OC)c3)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.68
2656	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(OC(F)(F)F)ccc3)c3ccccc13)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.89

Example No.	Structure	ESI-MS	Retention Time (min)
2657	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3cc(F)(F)F)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	4.85
2658	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccc(C(C)(C)C)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.8 (M + H)	5.15
2659	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccsc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.8 (M + H)	4.63
2660	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	4.61
2661	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccc(Cl)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.86
2662	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccc(Br)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.64

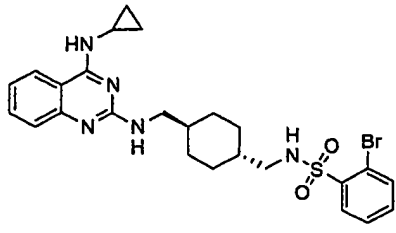
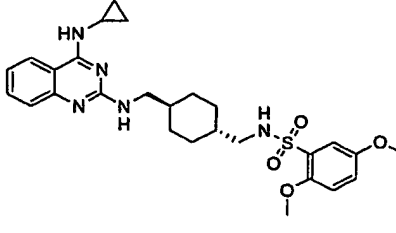
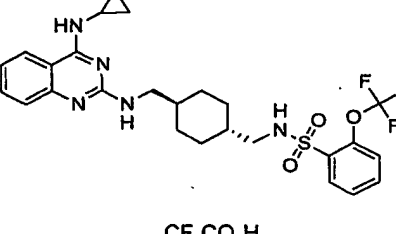
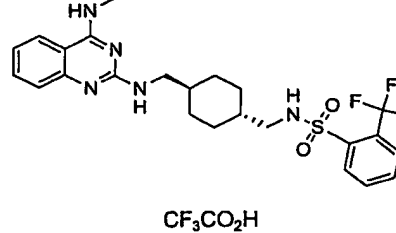
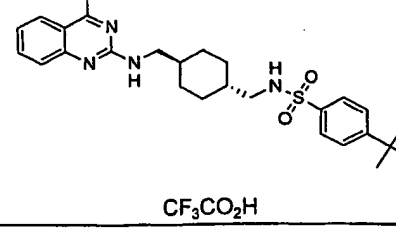
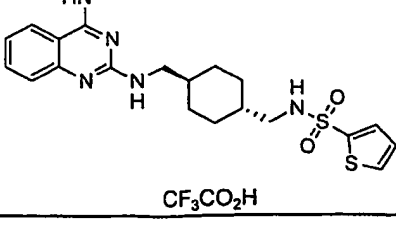
Example No.	Structure	ESI-MS	Retention Time (min)
2663	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(Cl)cc(Cl)c3)C3=CC=CC=C3.CC(F)(F)C(=O)O</chem>	536.4 (M + H)	4.81
2664	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(Br)cc(OC(F)(F)F)c3)C3=CC=CC=C3.CC(F)(F)C(=O)O</chem>	630.4 (M + H)	4.85
2665	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(F)c(F)c(F)c3)C3=CC=CC=C3.CC(F)(F)C(=O)O</chem>	604.6 (M + H)	4.87
2666	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cccc4ccccc34)C3=CC=CC=C3.CC(F)(F)C(=O)O</chem>	518.6 (M + H)	4.67
2667	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cccc4ccccc34)C3=CC=CC=C3.CC(F)(F)C(=O)O</chem>	518.6 (M + H)	4.90
2668	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cccc4ccccc34N(C)C)C3=CC=CC=C3.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	561.6 (M + H)	4.64

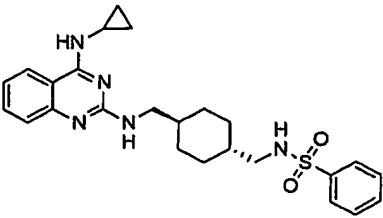
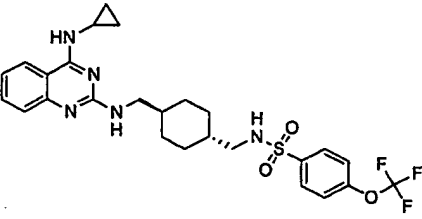
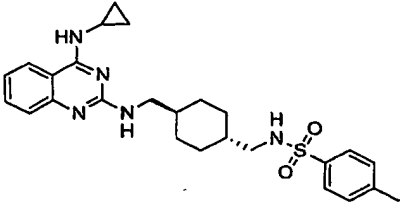
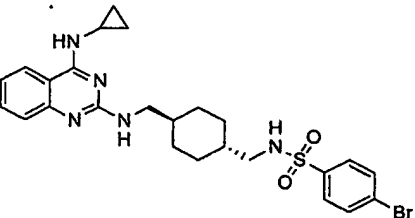
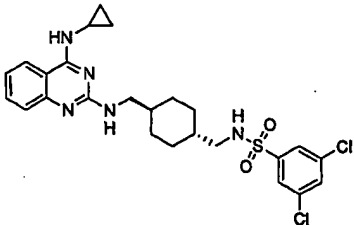
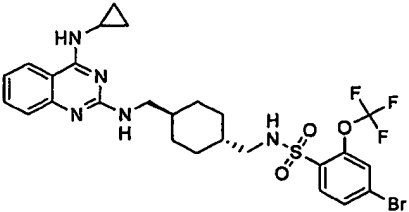
Example No.	Structure	ESI-MS	Retention Time (min)
2669	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccccc3F)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.73
2670	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccc(F)cc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.74
2671	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccccc3Cl)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.89
2672	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccc(Cl)cc3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.93
2673	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3ccccc3Br)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.0 (M + H)	4.89
2674	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN(C1)CNS(=O)(=O)c3cc(OC)cc(OC)c3)cc3ccccc13</chem> $\text{CF}_3\text{CO}_2\text{H}$	542.8 (M + H)	4.76

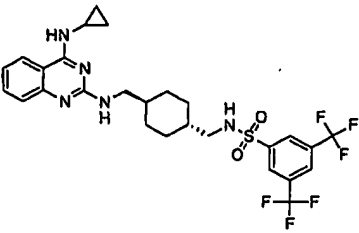
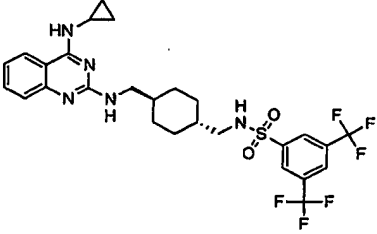
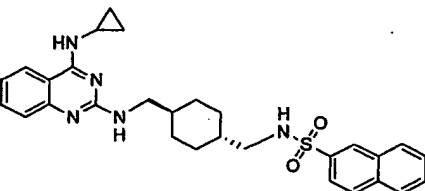
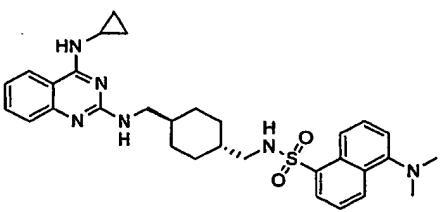
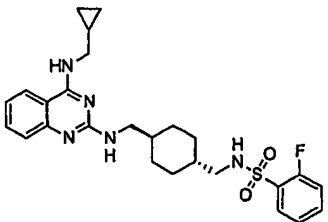
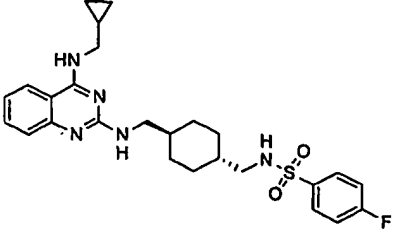
Example No.	Structure	ESI-MS	Retention Time (min)
2675	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.03
2676	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.96
2677	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC4=CC=C(C(C)(C)C)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.8 (M + H)	5.25
2678	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC4=CC=C(S)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.67
2679	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.71
2680	 <chem>CC(C)(C)Nc1ncnc2c1cccnc2CNC3CCCCC3NS(=O)(=O)OC4=CC=C(Cl)C=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.95

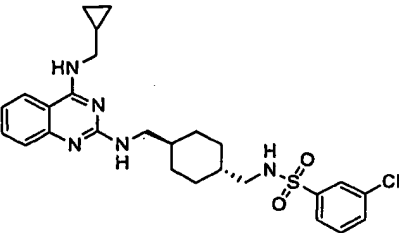
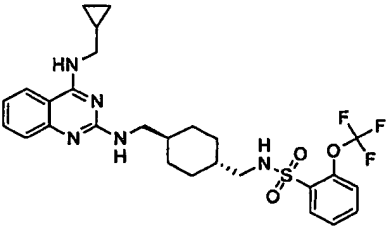
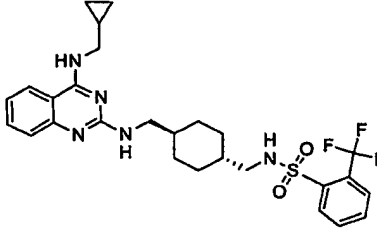
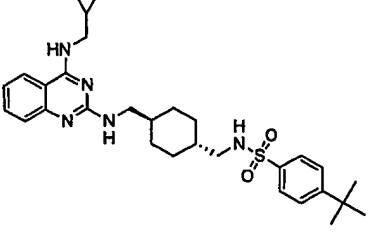
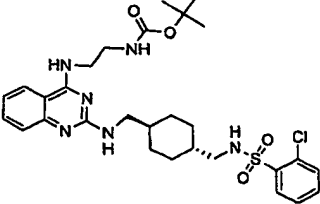
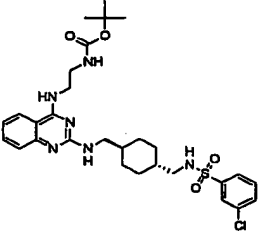
Example No.	Structure	ESI-MS	Retention Time (min)
2681	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2ccc(OC(F)(F)F)cc2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	566.8 (M + H)	5.07
2682	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2ccc(C)cc2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	496.8 (M + H)	4.83
2683	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2ccc(Br)cc2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	560.6 (M + H)	5.01
2684	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2cc(Cl)cc(Cl)c2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	550.6 (M + H)	5.07
2685	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2cc(Br)cc(OC(F)(F)F)c2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	644.6 (M + H)	5.29
2686	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11</chem> <chem>CC1(C)CCN(C1)CCN(S(=O)(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)C1</chem> <chem>CC(C)(C)Nc1nc2c(ncn2C1CCN1)cccc1ccccc11.CC(F)(F)F(=O)O</chem>	618.6 (M + H)	5.25

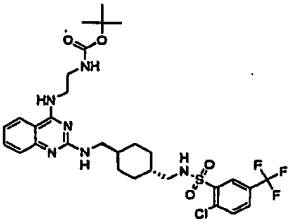
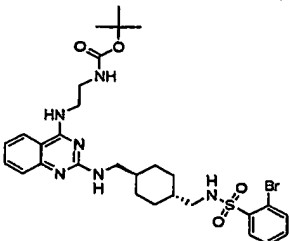
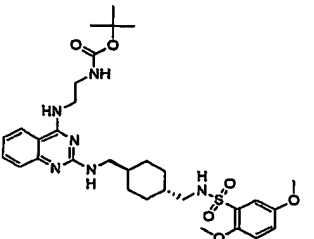
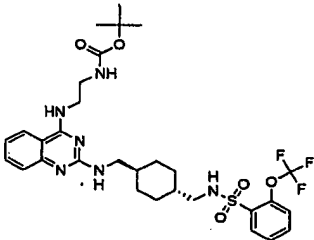
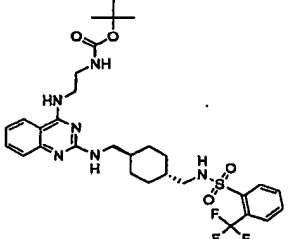
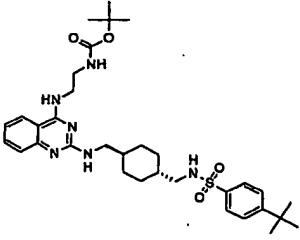
Example No.	Structure	ESI-MS	Retention Time (min)
2687	 <chem>CC(C)(C)Nc1nc2c(nc1c2)NCC[C@H]3CCCC[C@H]3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.01
2688	 <chem>CC(C)(C)Nc1nc2c(nc1c2)NCC[C@@H]3CCCC[C@H]3NS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.04
2689	 <chem>CC(C)(C)Nc1nc2c(nc1c2)NCC[C@H]3CCCC[C@H]3NS(=O)(=O)c4ccc(N(C)C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	575.8 (M + H)	4.75
2690	 <chem>C1CC1Nc2nc3c(nc2c3)NCC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc(F)ccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.6 (M + H)	4.51
2691	 <chem>C1CC1Nc2nc3c(nc2c3)NCC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc(Cl)ccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.59
2692	 <chem>C1CC1Nc2nc3c(nc2c3)NCC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cccc(Cl)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.71

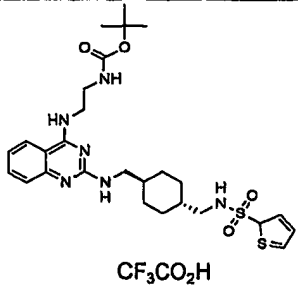
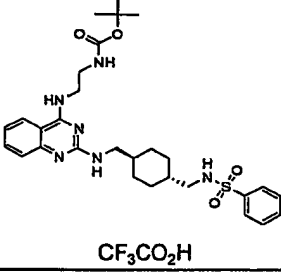
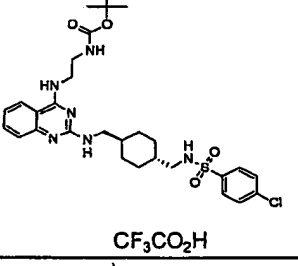
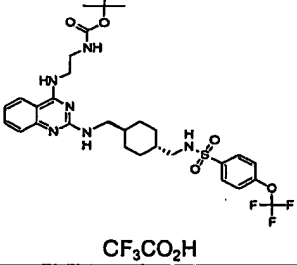
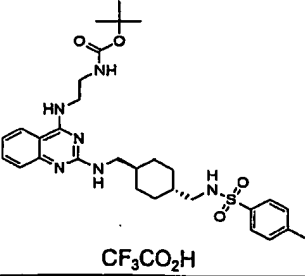
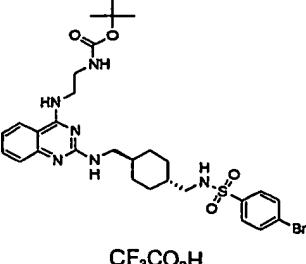
Example No.	Structure	ESI-MS	Retention Time (min)
2693	 <chem>BrC1=CC=C(C=C1)S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	4.63
2694	 <chem>COc1cc(OC)cc(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.8 (M + H)	4.55
2695	 <chem>FC(F)(F)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	4.79
2696	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.69
2697	 <chem>CC(C)(C)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	5.03
2698	 <chem>c1ccsc1S(=O)(=O)N[C@H]2CCCC[C@H]2CN3C(=N2)c4ccccc4N3C5CC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.43

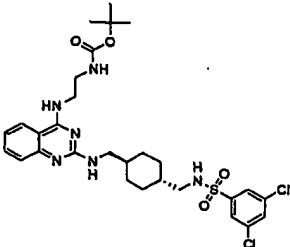
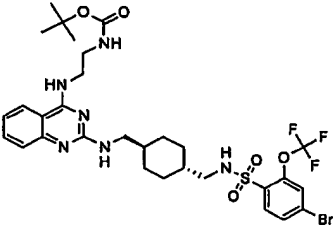
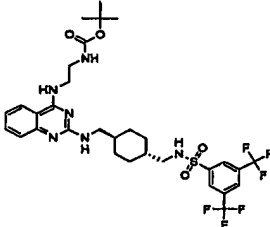
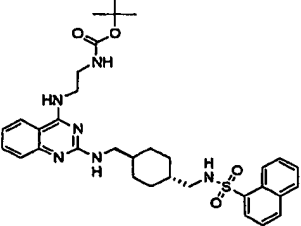
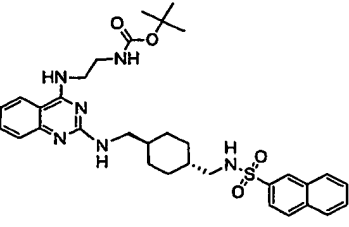
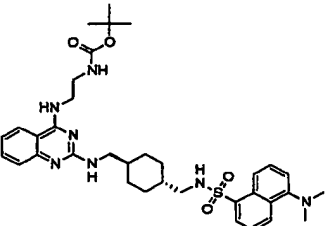
Example No.	Structure	ESI-MS	Retention Time (min)
2699	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.6 (M + H)	4.50
2700	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	4.87
2701	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(C)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.6 (M + H)	4.65
2702	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	4.75
2703	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5cc(Cl)cc(Cl)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.90
2704	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@@H]4CCCC[C@H]4NS(=O)(=O)c5cc(Br)cc(OC(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	628.6 (M + H)	5.08

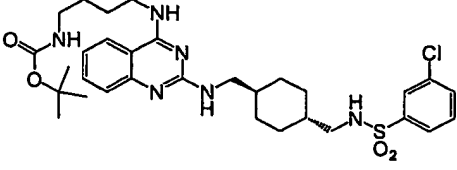
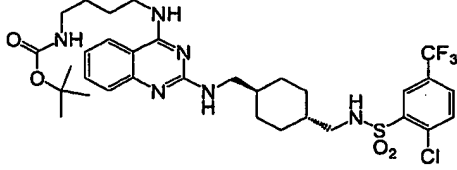
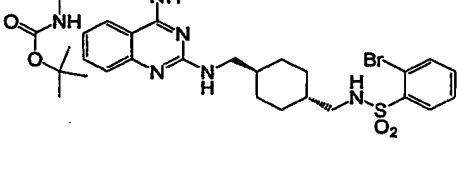
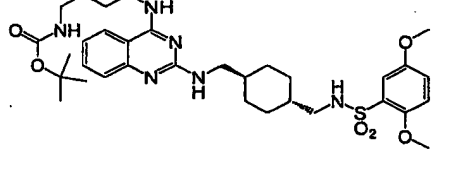
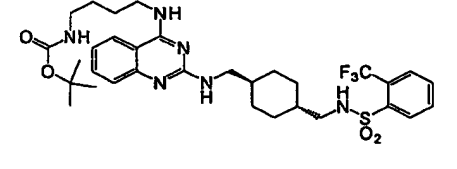
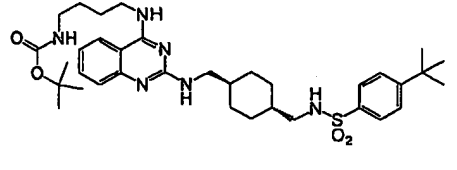
Example No.	Structure	ESI-MS	Retention Time (min)
2705	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5cc(F)c(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	602.6 (M + H)	5.10
2706	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5cc(F)c(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.71
2707	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc6ccccc6c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.81
2708	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc6cc(C)ccc6c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.50
2709	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccccc5F</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.64
2710	 <chem>CC1(C)Nc2nc3ccccc3n2NCC4CCCCC4NS(=O)(=O)c5ccc(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.73

Example No.	Structure	ESI-MS	Retention Time (min)
2711	 <chem>CC1(C)CN2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.8 (M + H)	4.87
2712	 <chem>CC1(C)CN2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4cc(F)(F)Fcc4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	4.93
2713	 <chem>CC1(C)CN2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4cc(F)(F)Fcc4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	548.6 (M + H)	4.87
2714	 <chem>CC1(C)CN2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	5.19
2715	 <chem>CC(C)(C)OC(=O)NCC1C2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.76
2716	 <chem>CC(C)(C)OC(=O)NCC1C2C(=N1)N(C2CC3CCCCC3NS(=O)(=O)c4cccc(Cl)c4)CC5C6C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.4 (M + H)	4.87

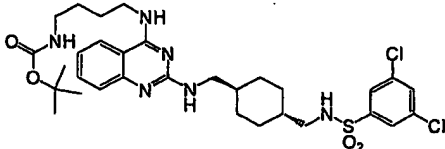
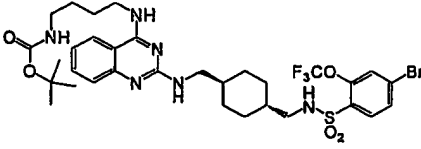
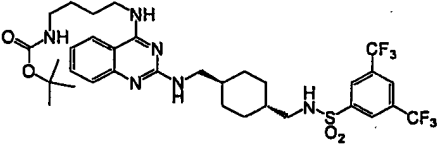
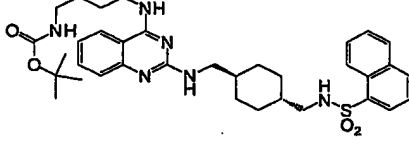
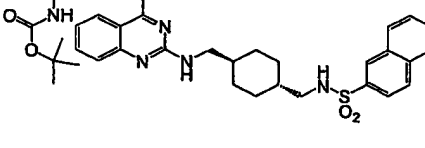
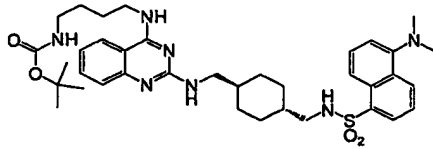
Example No.	Structure	ESI-MS	Retention Time (min)
2717	 $\text{CF}_3\text{CO}_2\text{H}$	671.6 (M + H)	5.05
2718	 $\text{CF}_3\text{CO}_2\text{H}$	647.6 (M + H)	4.79
2719	 $\text{CF}_3\text{CO}_2\text{H}$	629.8 (M + H)	4.67
2720	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	4.91
2721	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	4.85
2722	 $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	5.14

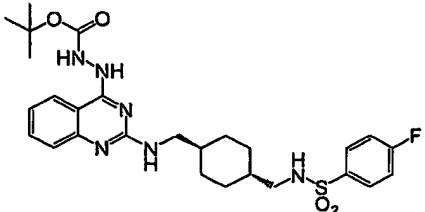
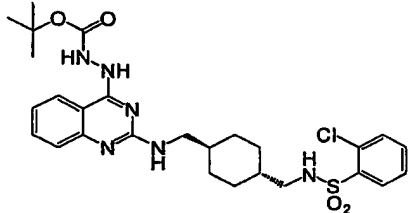
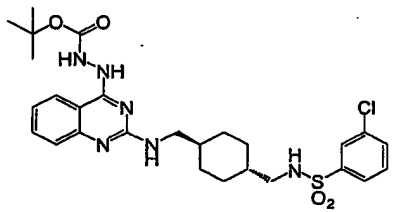
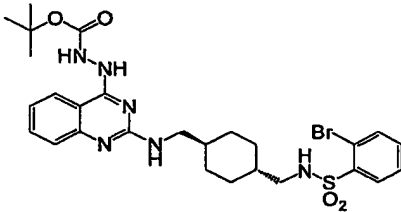
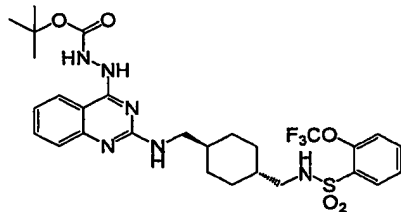
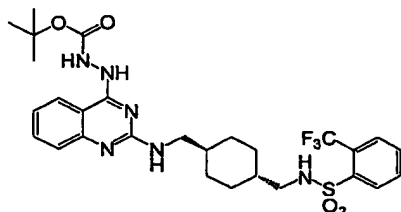
Example No.	Structure	ESI-MS	Retention Time (min)
2723	 $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.63
2724	 $\text{CF}_3\text{CO}_2\text{H}$	569.8 (M + H)	4.66
2725	 $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.88
2726	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.01
2727	 $\text{CF}_3\text{CO}_2\text{H}$	583.8 (M + H)	4.77
2728	 $\text{CF}_3\text{CO}_2\text{H}$	647 (M + H)	4.92

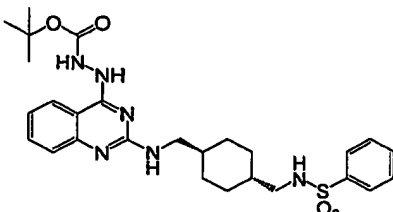
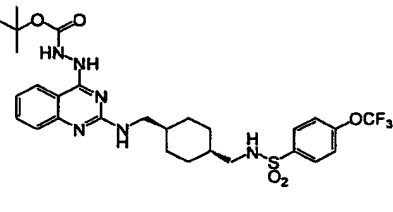
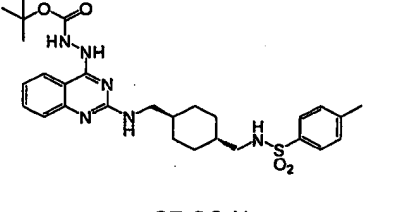
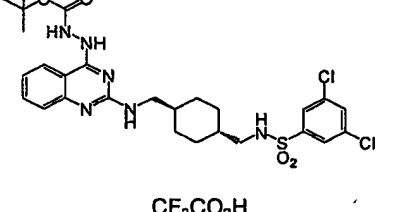
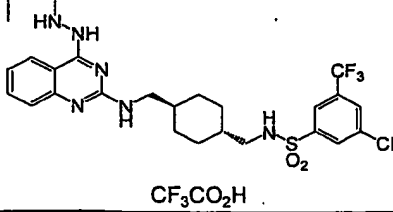
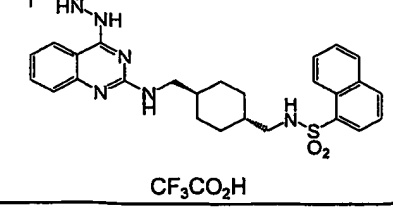
Example No.	Structure	ESI-MS	Retention Time (min)
2729	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	5.13
2730	 $\text{CF}_3\text{CO}_2\text{H}$	731.6 (M + H)	5.19
2731	 $\text{CF}_3\text{CO}_2\text{H}$	705.8 (M + H)	5.22
2732	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.91
2733	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.93
2734	 $2\text{CF}_3\text{CO}_2\text{H}$	663.0 (M + H)	4.67

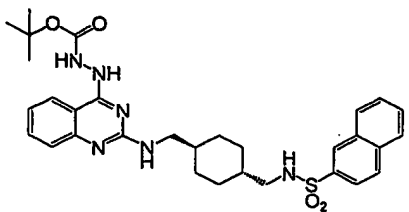
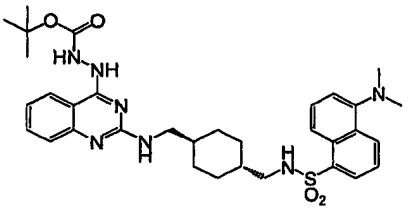
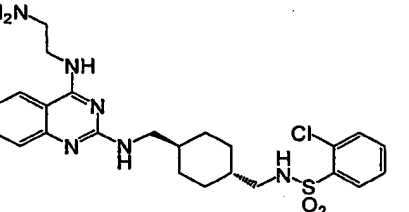
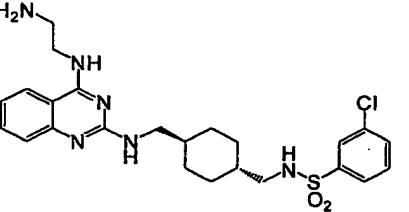
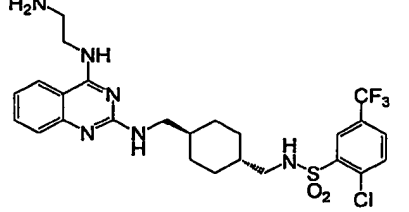
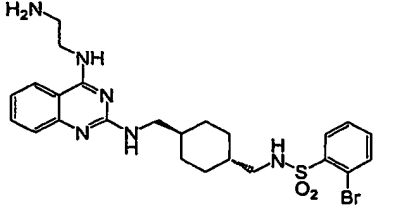
Example No.	Structure	ESI-MS	Retention Time (min)
2735	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC=C(Cl)C=C5)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	631.8 (M + H)	5.01
2736	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC(=C(C(F)(F)F))C=C5Cl)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	699.0 (M + H)	5.19
2737	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC=C(Br)C=C5)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	675.8 (M + H)	4.95
2738	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC(OC)=CC(OC)=C5)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	657.8 (M + H)	4.81
2739	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC=C(C(F)(F)F)C=C5)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	4.97
2740	 <chem>CC(C)(C)OC(=O)Nc1ccc2nc(NC3CCCCC3/C=C/N4C=CC(=C4)S(=O)(=O)C5=CC=C(C(C)(C)C)C=C5)nc2cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.27

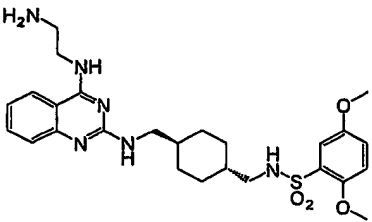
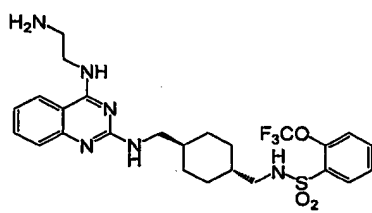
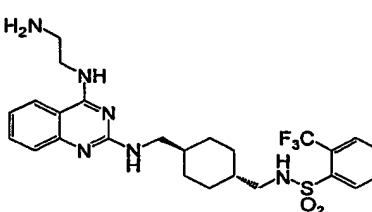
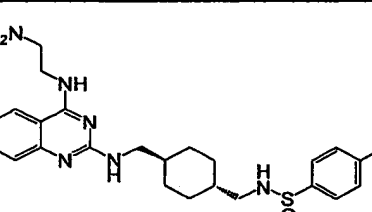
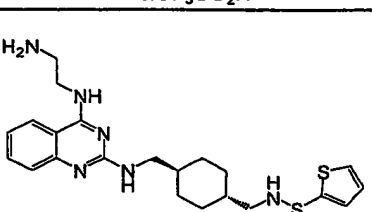
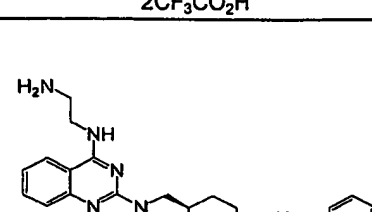
Example No.	Structure	ESI-MS	Retention Time (min)
2741	<p>CF₃CO₂H</p>	603.4 (M + H)	4.77
2742	<p>CF₃CO₂H</p>	597.8 (M + H)	4.79
2743	<p>CF₃CO₂H</p>	631.8 (M + H)	5.02
2744	<p>CF₃CO₂H</p>	681.8 (M + H)	5.14
2745	<p>CF₃CO₂H</p>	611.8 (M + H)	4.93
2746	<p>CF₃CO₂H</p>	675.0 (M + H)	5.05

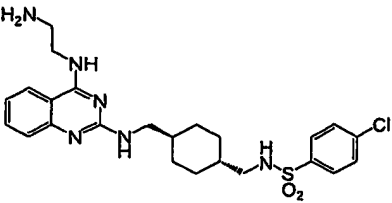
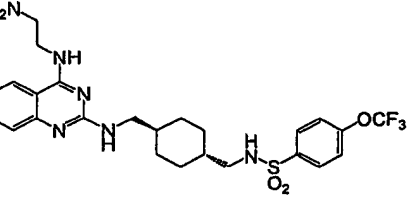
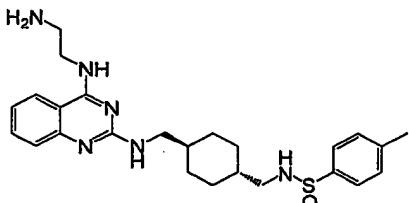
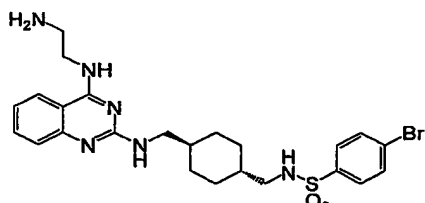
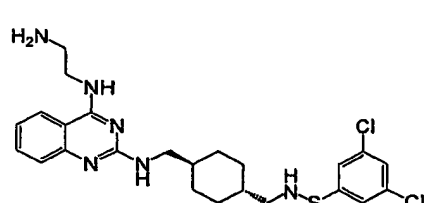
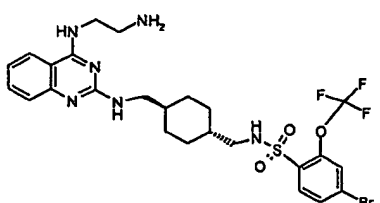
Example No.	Structure	ESI-MS	Retention Time (min)
2747	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cc(Cl)cc(Cl)c6</chem> $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	5.29
2748	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cc(Br)cc(OC(F)(F)F)c6</chem> $\text{CF}_3\text{CO}_2\text{H}$	759.6 (M + H)	5.31
2749	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cc(C(F)(F)F)cc(C(F)(F)F)c6</chem> $\text{CF}_3\text{CO}_2\text{H}$	733.8 (M + H)	5.36
2750	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cccc7ccccc67</chem> $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.05
2751	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cccc7ccccc67</chem> $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.08
2752	 <chem>CC1(C)OC(=O)N1c2nc3c(nc2N)N(CCN3)Nc4ccc(cc4)Nc5ccccc5S(=O)(=O)c6cccc7c(C)ccc67</chem> $2\text{CF}_3\text{CO}_2\text{H}$	691.0 (M + H)	4.89

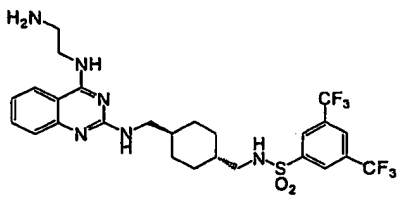
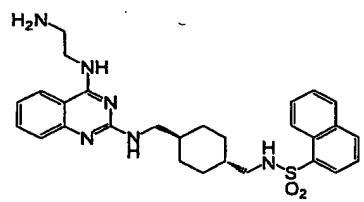
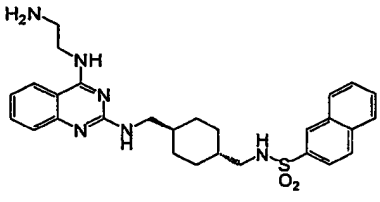
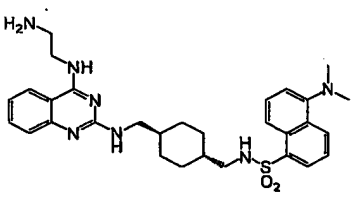
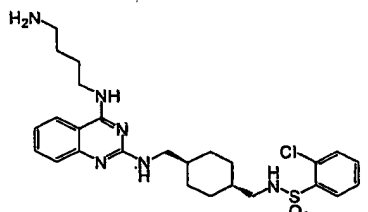
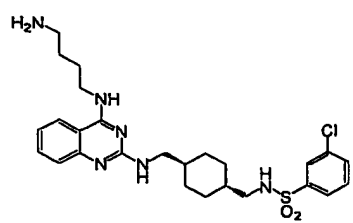
Example No.	Structure	ESI-MS	Retention Time (min)
2753	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)F)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.51
2754	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)Cl)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.57
2755	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)Cl)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.69
2756	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)Br)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	619.6 (M + H)	4.63
2757	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)C(F)(F)F)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.72
2758	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1CNCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)C5=CC=C(C=C5)C(F)(F)F)cc6ccccc16</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.67

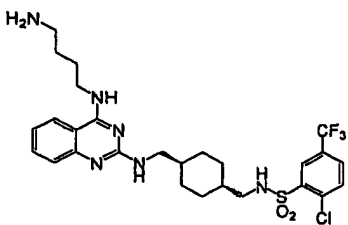
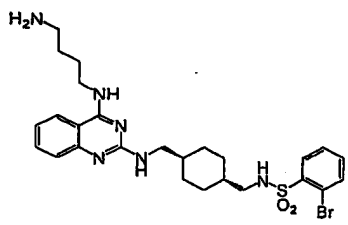
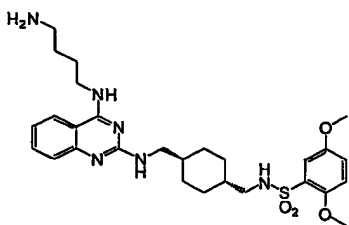
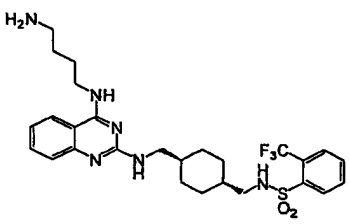
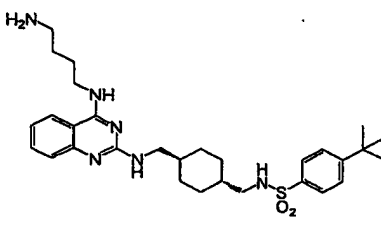
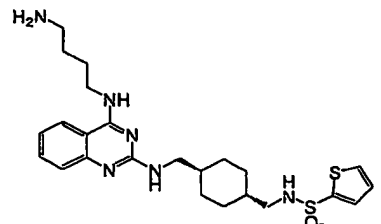
Example No.	Structure	ESI-MS	Retention Time (min)
2759	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	541.8 (M + H)	4.45
2760	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.38
2761	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4ccc(C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	555.8 (M + H)	4.57
2762	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.94
2763	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	677.8 (M + H)	5.05
2764	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CS(=O)(=O)c4c5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.73

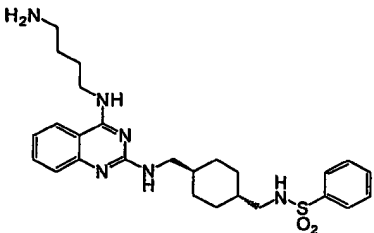
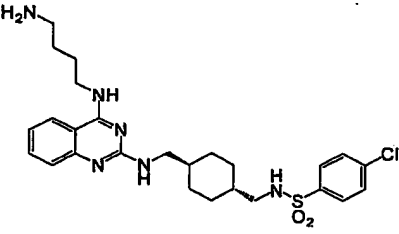
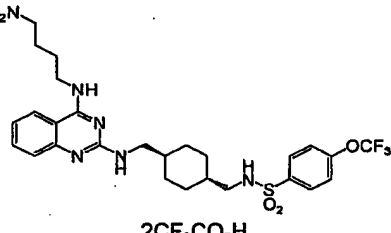
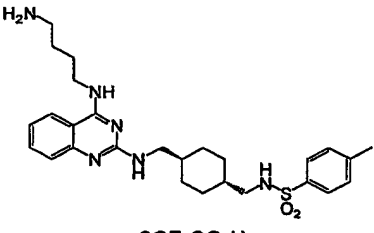
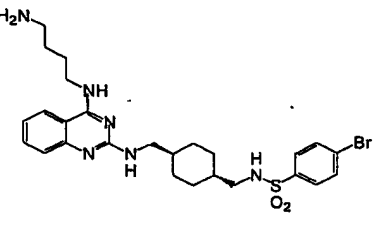
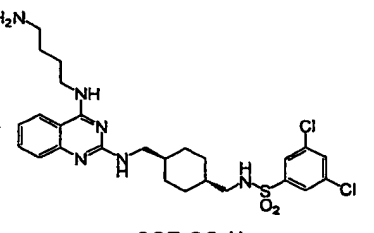
Example No.	Structure	ESI-MS	Retention Time (min)
2765	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=CC=C4S(=O)(=O)N)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.75
2766	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(C=C4)N(C)C)S(=O)(=O)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	635.0 (M + H)	4.47
2767	 <chem>NCCNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(Cl)C=C4S(=O)(=O)N)cc5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.83
2768	 <chem>NCCNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(Cl)C=C4S(=O)(=O)N)cc5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.99
2769	 <chem>NCCNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(Cl)C(=C4)C(F)(F)F)S(=O)(=O)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.16
2770	 <chem>NCCNc1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=C(Br)C=C4S(=O)(=O)N)cc5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	3.85

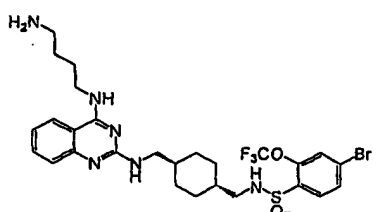
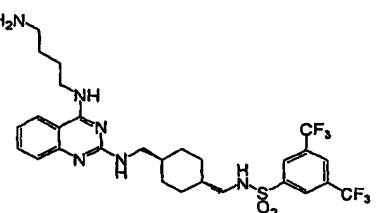
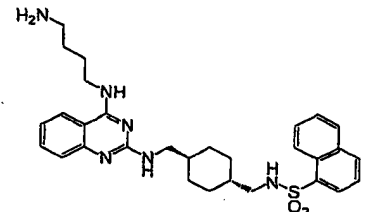
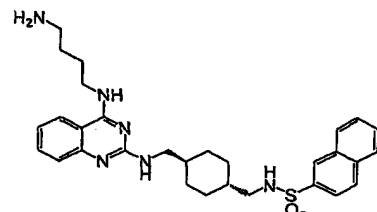
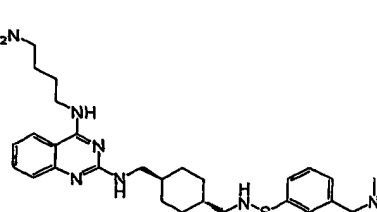
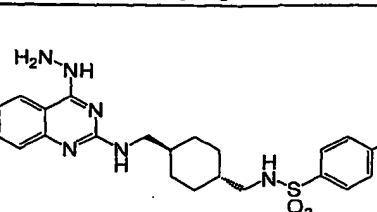
Example No.	Structure	ESI-MS	Retention Time (min)
2771	 <chem>COc1cc(OC)cc(S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	529.6 (M + H)	3.75
2772	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	553.8 (M + H)	3.99
2773	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	537.6 (M + H)	3.93
2774	 <chem>CC(C)(C)c1ccc(S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	525.8 (M + H)	4.22
2775	 <chem>c1ccsc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	3.64
2776	 <chem>c1ccccc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	469.6 (M + H)	3.71

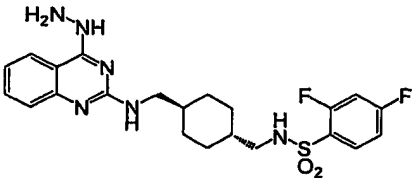
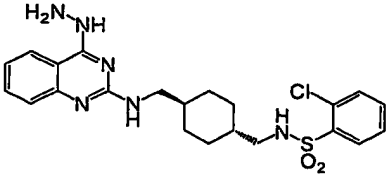
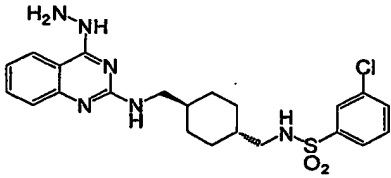
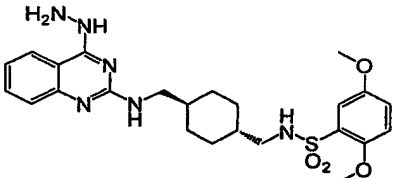
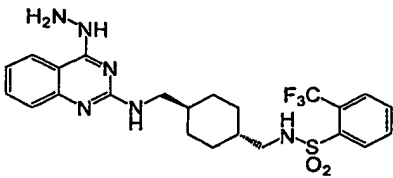
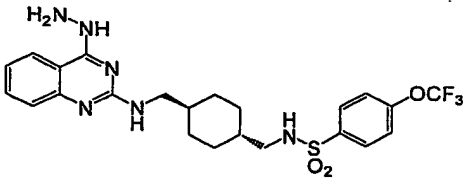
Example No.	Structure	ESI-MS	Retention Time (min)
2777	 <chem>2CF3CO2H</chem>	503.6 (M + H)	3.97
2778	 <chem>2CF3CO2H</chem>	553.8 (M + H)	4.17
2779	 <chem>2CF3CO2H</chem>	483.4 (M + H)	3.87
2780	 <chem>2CF3CO2H</chem>	547.6 (M + H)	4.04
2781	 <chem>2CF3CO2H</chem>	537.4 (M + H)	4.23
2782	 <chem>2CF3CO2H</chem>	631.6 (M + H)	4.23

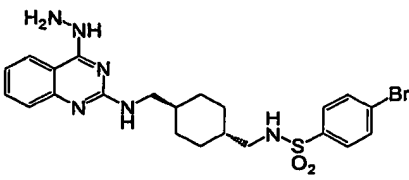
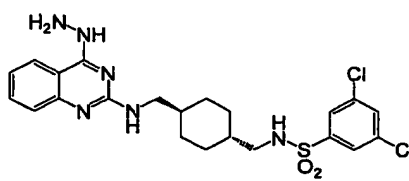
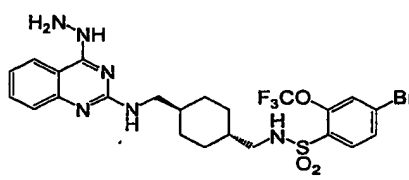
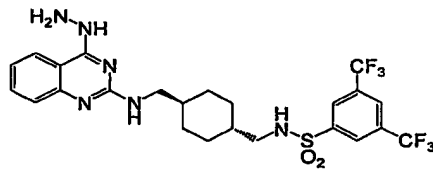
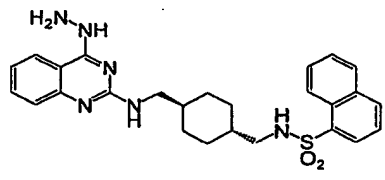
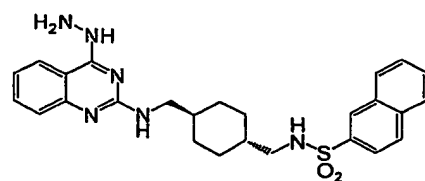
Example No.	Structure	ESI-MS	Retention Time (min)
2783	 $2\text{CF}_3\text{CO}_2\text{H}$	605.8 (M + H)	4.41
2784	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.01
2785	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.07
2786	 $3\text{CF}_3\text{CO}_2\text{H}$	562.6 (M + H)	3.77
2787	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	3.90
2788	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	4.04

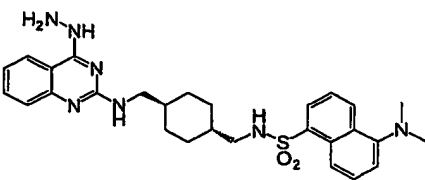
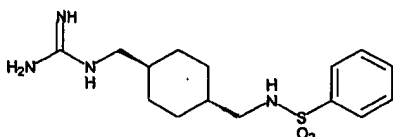
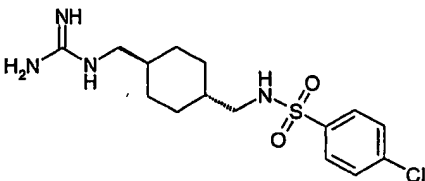
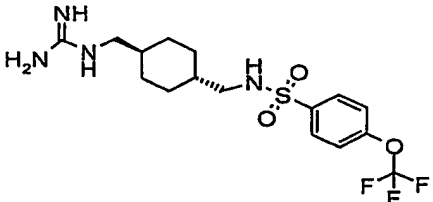
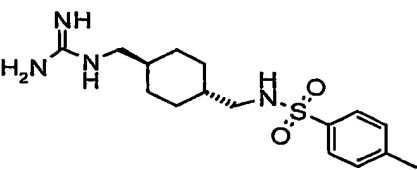
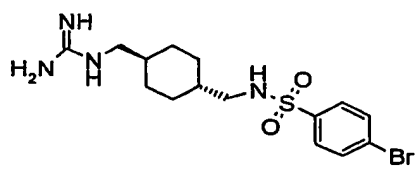
Example No.	Structure	ESI-MS	Retention Time (min)
2789	 <chem>2CF3CO2H</chem>	599.6 (M + H)	4.24
2790	 <chem>2CF3CO2H</chem>	575.0 (M + H)	3.95
2791	 <chem>2CF3CO2H</chem>	557.6 (M + H)	3.86
2792	 <chem>2CF3CO2H</chem>	565.6 (M + H)	4.03
2793	 <chem>2CF3CO2H</chem>	554 (M + H)	4.29
2794	 <chem>2CF3CO2H</chem>	503.6 (M + H)	3.78

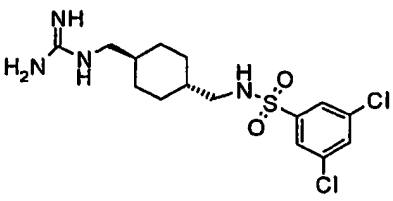
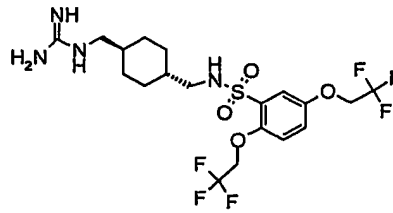
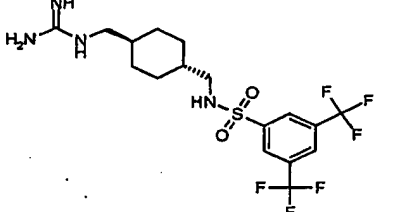
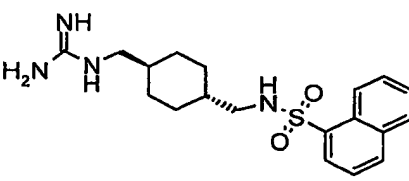
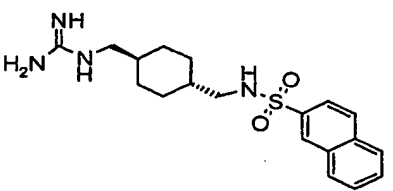
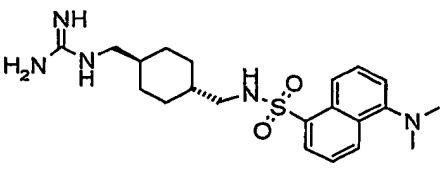
Example No.	Structure	ESI-MS	Retention Time (min)
2795	 $2\text{CF}_3\text{CO}_2\text{H}$	497.6 (M + H)	3.83
2796	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	4.05
2797	 $2\text{CF}_3\text{CO}_2\text{H}$	582.0 (M + H)	4.23
2798	 $2\text{CF}_3\text{CO}_2\text{H}$	511 (M + H)	3.95
2799	 $2\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.10
2800	 $2\text{CF}_3\text{CO}_2\text{H}$	565.0 (M + H)	4.32

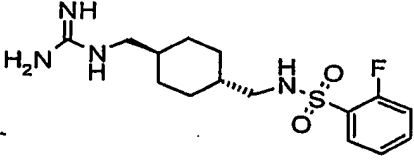
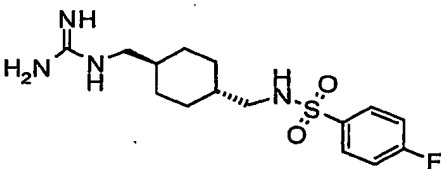
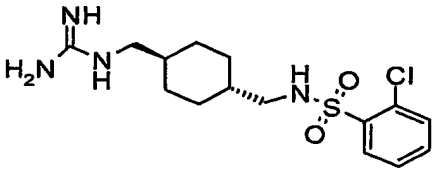
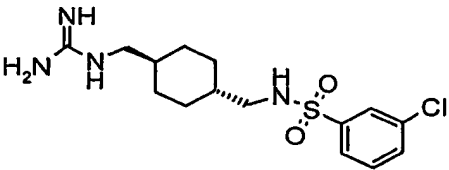
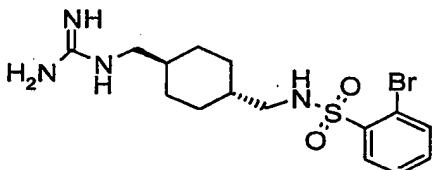
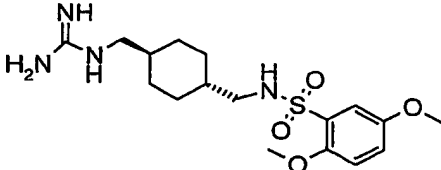
Example No.	Structure	ESI-MS	Retention Time (min)
2801	 <p>2CF₃CO₂H</p>	659.6 (M + H)	4.35
2802	 <p>2CF₃CO₂H</p>	634.0 (M + H)	4.43
2803	 <p>2CF₃CO₂H</p>	547.6 (M + H)	4.09
2804	 <p>2CF₃CO₂H</p>	547.6 (M + H)	4.15
2805	 <p>3CF₃CO₂H</p>	590.6 (M + H)	3.93
2806	 <p>2CF₃CO₂H</p>	459.6 (M + H)	4.07

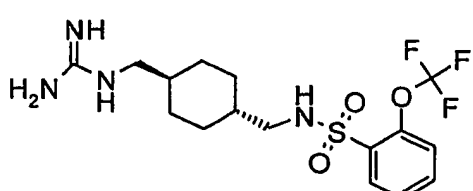
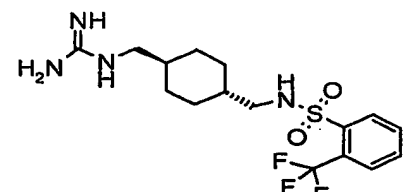
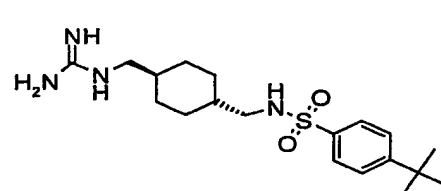
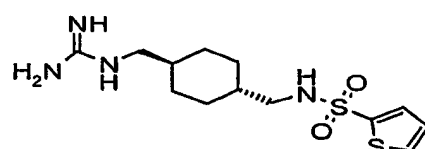
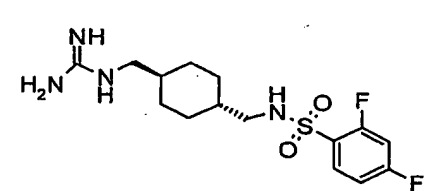
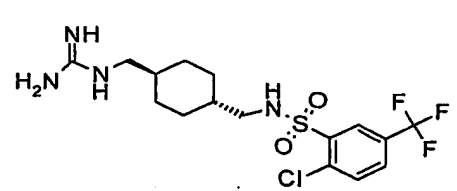
Example No.	Structure	ESI-MS	Retention Time (min)
2807	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4cc(F)cc(F)c4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.6 (M + H)	4.07
2808	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccccc4Cl)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.07
2809	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4cccc(Cl)c4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.23
2810	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4cc(OC)cc(OC)c4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	501.8 (M + H)	4.15
2811	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccccc4C(F)(F)F)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.27
2812	 <chem>Nc1nc2c(ncn2C1CCN3CCSC(=O)c4ccc(OC(F)(F)F)cc4)CC3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	525.6 (M + H)	4.37

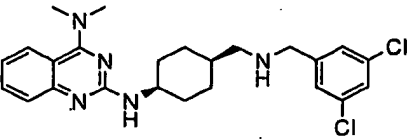
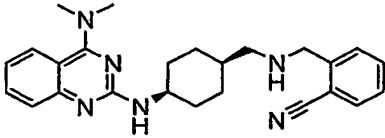
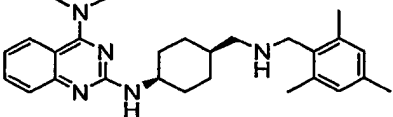
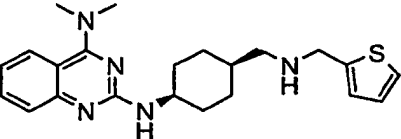
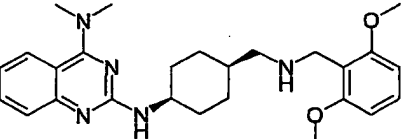
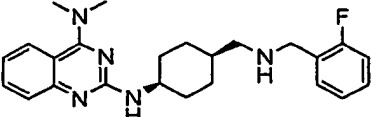
Example No.	Structure	ESI-MS	Retention Time (min)
2813	 <chem>BrC1=CC=C(S(=O)(=O)NCC2(CCCC(CC2)CN3C=NC4=CC=CC=C4N3NN)CC3)C=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.25
2814	 <chem>ClC1=CC(=C(C=C1)S(=O)(=O)NCC2(CCCC(CC2)CN3C=NC4=CC=CC=C4N3NN)CC3)C(Cl)=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.49
2815	 <chem>BrC1=CC(=C(C=C1)S(=O)(=O)NCC2(CCCC(CC2)CN3C=NC4=CC=CC=C4N3NN)CC3)C(OC(F)(F)F)=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	603.0 (M + H)	4.60
2816	 <chem>FC(F)(F)C1=CC(=C(C=C1)S(=O)(=O)NCC2(CCCC(CC2)CN3C=NC4=CC=CC=C4N3NN)CC3)C(C(F)(F)F)=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	577.6 (M + H)	4.72
2817	 <chem>c1ccc2cc(S(=O)(=O)NCC3(CCCC(CC3)CN4C=NC5=CC=CC=C5N4NN)CC4)ccc2c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491 (M + H)	4.31
2818	 <chem>c1ccc2cc(S(=O)(=O)NCC3(CCCC(CC3)CN4C=NC5=CC=CC=C5N4NN)CC4)ccc2c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491.6 (M + H)	4.33

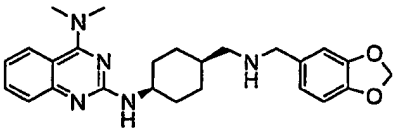
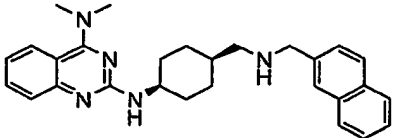
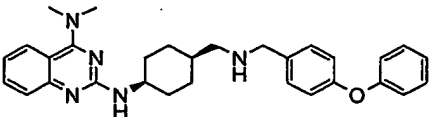
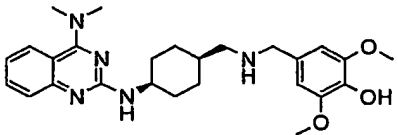
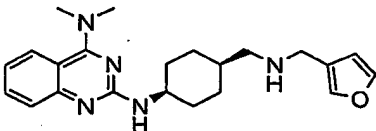
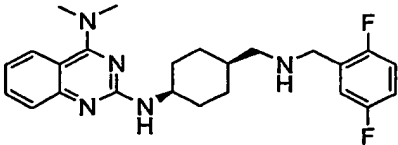
Example No.	Structure	ESI-MS	Retention Time (min)
2819	 <chem>CC1=CC=C2C(=C1)C(=CC=C2)S(=O)(=O)NCC3CCCCC3CNc4nc5ccccc5n4NN</chem> $3\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.01
2820	 <chem>Nc1nc(NC2CCCCC2NS(=O)(=O)c3ccccc3)cc1</chem> 2HCl	325.4 (M + H)	3.91
2821	 <chem>Clc1ccc(S(=O)(=O)NCC2CCCCC2NC(=N)N)cc1</chem> 2HCl	359.4 (M + H)	4.24
2822	 <chem>COc1ccc(S(=O)(=O)NCC2CCCCC2NC(=N)N)cc1F(F)F</chem> 2HCl	409.4 (M + H)	4.51
2823	 <chem>Cc1ccc(S(=O)(=O)NCC2CCCCC2NC(=N)N)cc1</chem> 2HCl	339.6 (M + H)	4.09
2824	 <chem>BrC1=CC=C(S(=O)(=O)NCC2CCCCC2NC(=N)N)C=C1</chem> 2HCl	403.4 (M + H)	4.28

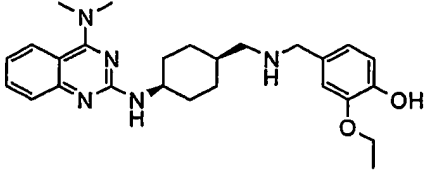
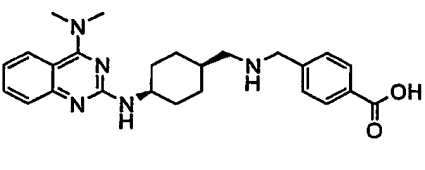
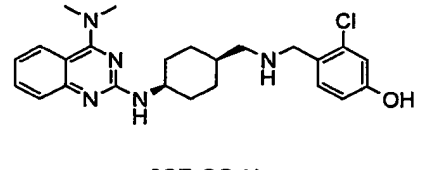
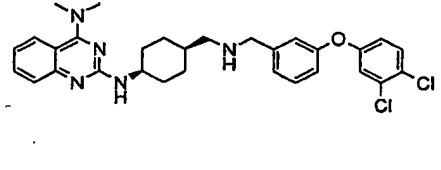
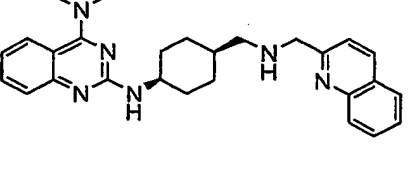
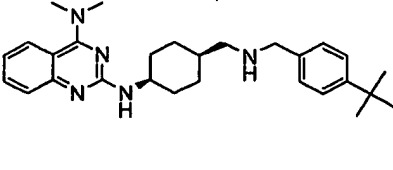
Example No.	Structure	ESI-MS	Retention Time (min)
2825	 2HCl	393.0 (M + H)	4.57
2826	 2HCl	521.6 (M + H)	4.69
2827	 2HCl	461.6 (M + H)	4.77
2828	 2HCl	375.4 (M + H)	4.33
2829	 2HCl	375.4 (M + H)	4.39
2830	 2HCl	418.8 (M + H)	4.33

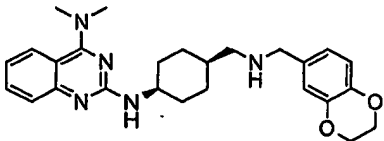
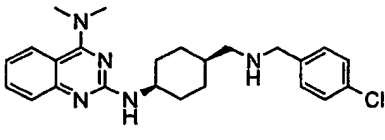
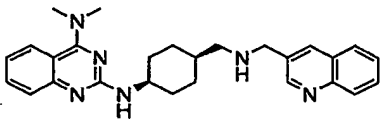
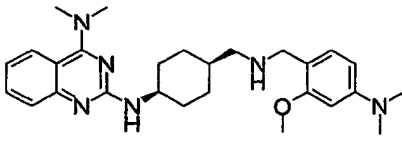
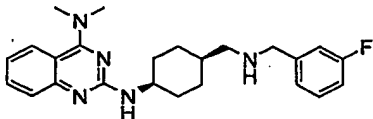
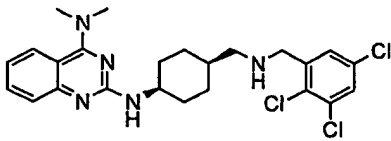
Example No.	Structure	ESI-MS	Retention Time (min)
2831	 2HCl	343.4 (M + H)	3.96
2832	 2HCl	343.4 (M + H)	4.03
2833	 2HCl	359.4 (M + H)	4.05
2834	 2HCl	359.4 (M + H)	4.24
2835	 2HCl	403.4 (M + H)	4.07
2836	 2HCl	385.4 (M + H)	4.00

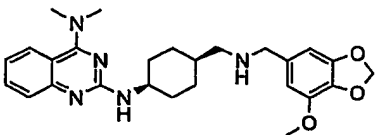
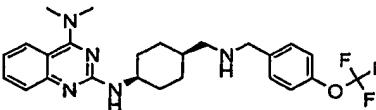
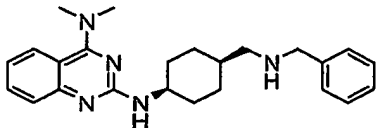
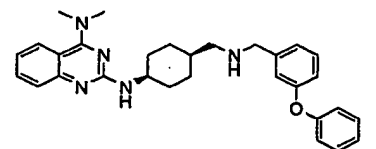
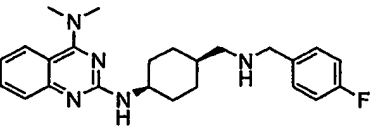
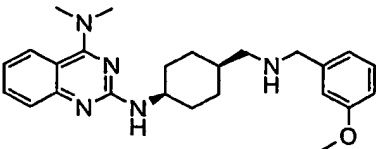
Example No.	Structure	ESI-MS	Retention Time (min)
2837	 2HCl	409.4 (M + H)	4.32
2838	 2HCl	393.6 (M + H)	4.23
2839	 2HCl	381.6 (M + H)	4.62
2840	 2HCl	330.8 (M + H)	3.83
2841	 2HCl	361.4 (M + H)	4.05
2842	 2HCl	427.4 (M + H)	4.51

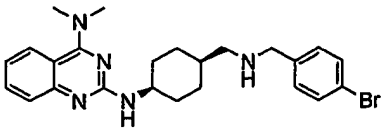
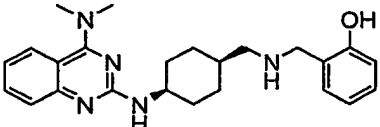
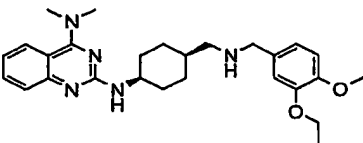
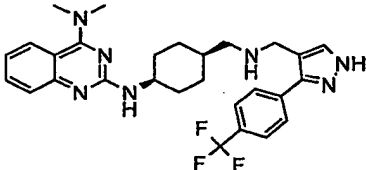
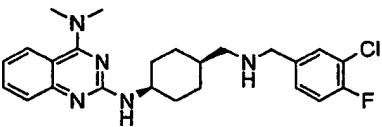
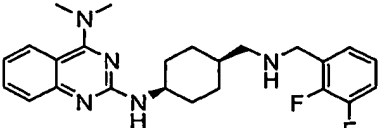
Example No.	Structure	ESI-MS	Retention Time (min)
2843	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=CC(=CC=C4)Cl</chem> <chem>2CF3CO2H</chem>	458.4 (M + H)	3.22
2844	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=CC=C5C(=CC=C4N5)C#N</chem> <chem>2CF3CO2H</chem>	415.4 (M + H)	3.01
2845	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=C(C)C(=CC(=C4)C)C</chem> <chem>2CF3CO2H</chem>	432.6 (M + H)	3.26
2846	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=CC=C5C(=CC=C4S5)</chem> <chem>2CF3CO2H</chem>	396.2 (M + H)	2.81
2847	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=CC(=CC=C4)OC</chem> <chem>2CF3CO2H</chem>	450.0 (M + H)	3.09
2848	 <chem>CC1=CN2C(=N1)N(C)C=N2[C@H]3CCCC[C@H]3CNCC4=CC(=CC=C4)F</chem> <chem>2CF3CO2H</chem>	408.4 (M + H)	2.85

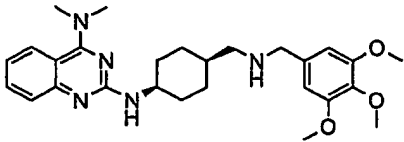
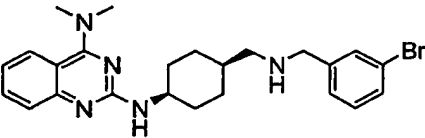
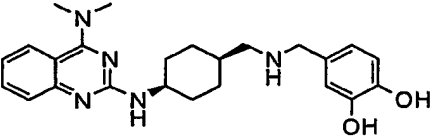
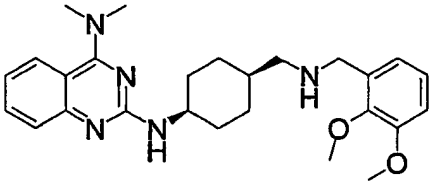
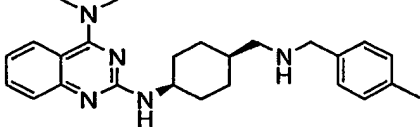
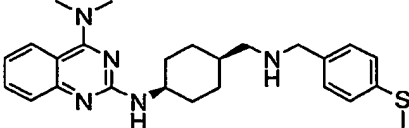
Example No.	Structure	ESI-MS	Retention Time (min)
2849	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4ccc(OC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.89
2850	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4c5ccccc5cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.20
2851	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4ccc(Oc5ccccc5)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
2852	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4cc(OC)c(O)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.71
2853	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4ccoc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.72
2854	 <chem>CN(C)c1nc2c(ncnc2n1)N[C@H]3CCCC[C@H]3NCNCCc4cc(F)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.91

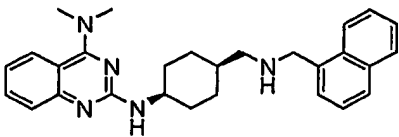
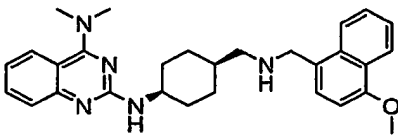
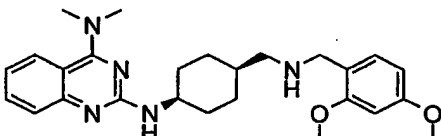
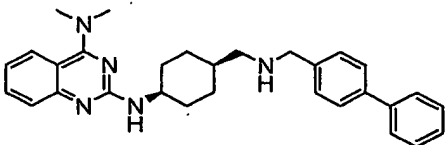
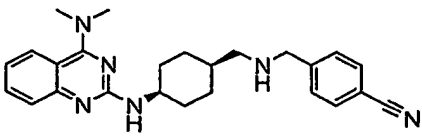
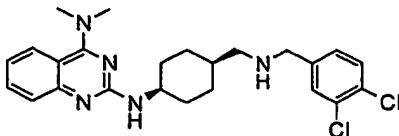
Example No.	Structure	ESI-MS	Retention Time (min)
2855	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3ccc(OCC)cc3)C3=CC=CC=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.82
2856	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3ccc(C(=O)O)cc3)C3=CC=CC=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.69
2857	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3cc(O)ccc3Cl)C3=CC=CC=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	2.85
2858	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3ccc(Oc4cc(Cl)cc(Cl)c4)cc3)C3=CC=CC=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	3.80
2859	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3ccc4c(n5cnc6ccccc56)ncn34)C3=CC=CC=C3</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.03
2860	 <chem>CCN(C)C1=NC2=CC=CC=C2N=C(NC1CCN(CCC1)NCCc3ccc(C(C)(C)C)cc3)C3=CC=CC=C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	3.41

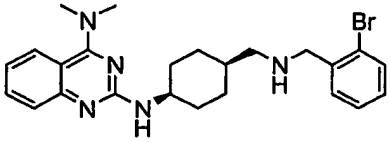
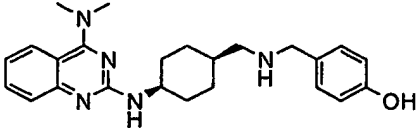
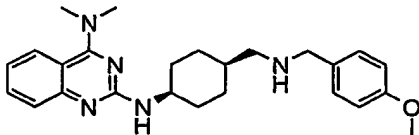
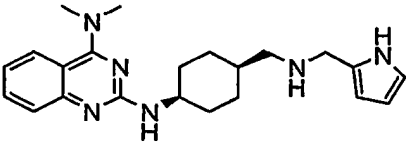
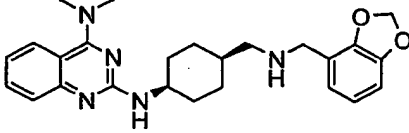
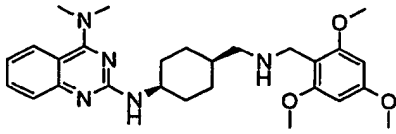
Example No.	Structure	ESI-MS	Retention Time (min)
2861	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4ccc5c(c4)OCCO5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.91
2862	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.05
2863	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4cnc5ccccc45</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.68
2864	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(N(C)C)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	463.4 (M + H)	2.76
2865	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4ccc(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2866	 <chem>CN(C)c1nc2c(ncnc2c1)N[C@H]3CCCC[C@H]3CNCCc4cc(Cl)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.30

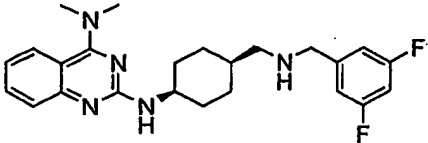
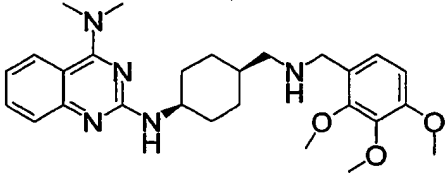
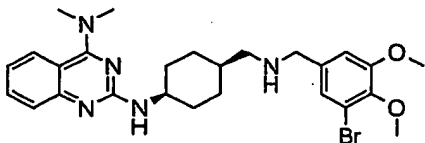
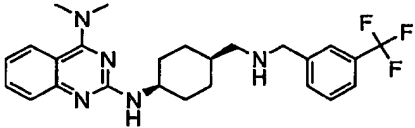
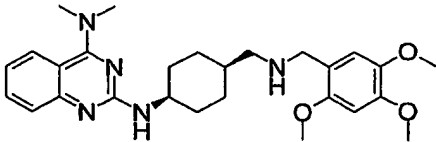
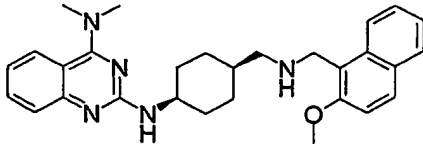
Example No.	Structure	ESI-MS	Retention Time (min)
2867	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(OC)=C5C(=C4)OCO5)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.93
2868	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(OC(F)(F)F)=CC=C4)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.27
2869	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC=CC=C4)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.6 (M + H)	2.88
2870	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(OC5=CC=CC=C5)=CC=C4)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.43
2871	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(F)=CC=C4)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2872	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(OC)=CC=C4)c4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.91

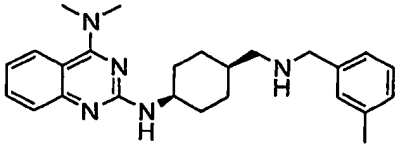
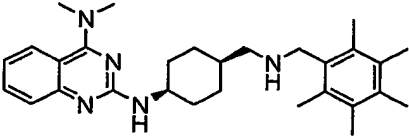
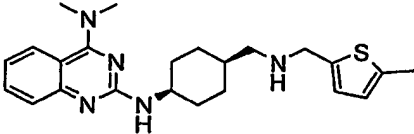
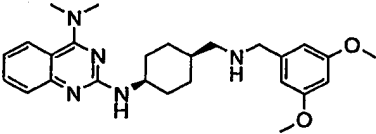
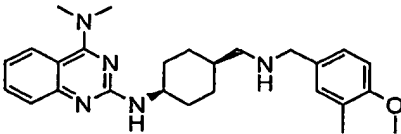
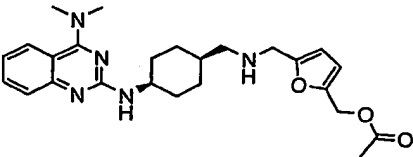
Example No.	Structure	ESI-MS	Retention Time (min)
2873	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5ccc(Br)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.09
2874	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5ccc(O)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
2875	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(OC)c(OC)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.97
2876	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5c[nH]c6c5ccc(cc6)C(F)(F)F</chem> $3\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.12
2877	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(F)c(Cl)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	3.10
2878	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(F)c(F)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.90

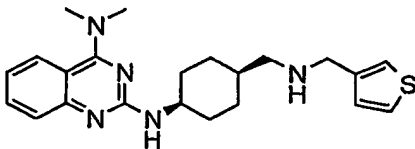
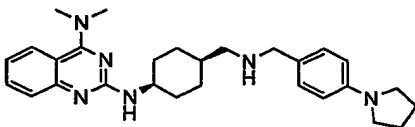
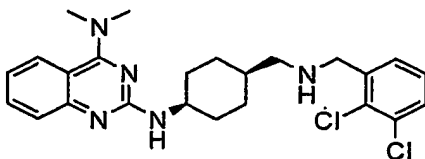
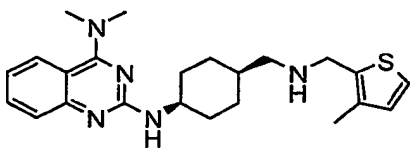
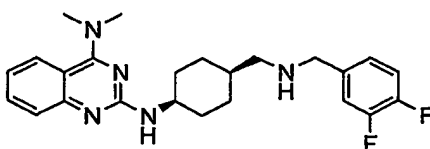
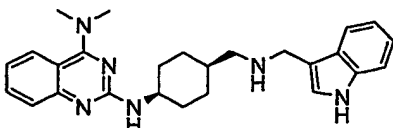
Example No.	Structure	ESI-MS	Retention Time (min)
2879	 <chem>COc1cc(OC)c(OC)cc1NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.89
2880	 <chem>BrC1=CC=C(C=C1)NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.07
2881	 <chem>Oc1cc(O)ccc1NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.4 (M + H)	2.61
2882	 <chem>COc1cc(OC)ccc1NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.93
2883	 <chem>Cc1ccc(cc1)NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.6 (M + H)	3.01
2884	 <chem>Ic1ccc(cc1)NC[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.08

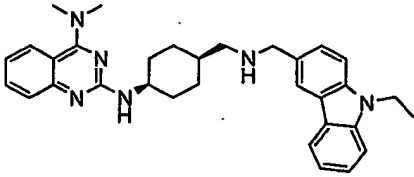
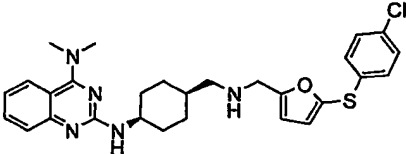
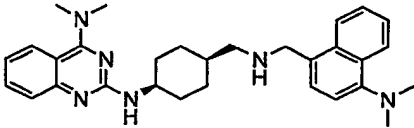
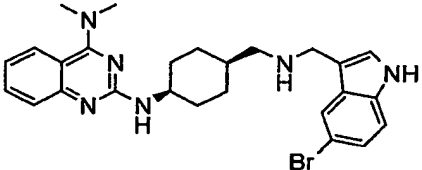
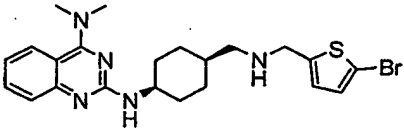
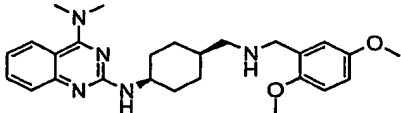
Example No.	Structure	ESI-MS	Retention Time (min)
2885	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc5ccccc5cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.18
2886	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.25
2887	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)ccc4OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.01
2888	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(cc4)-c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.40
2889	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(C#N)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.83
2890	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(Cl)cc(Cl)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.25

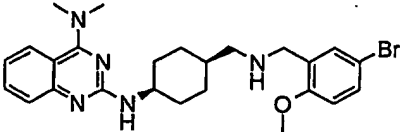
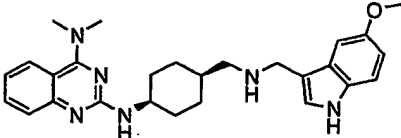
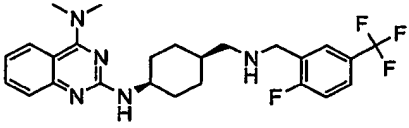
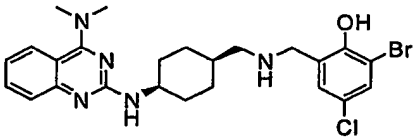
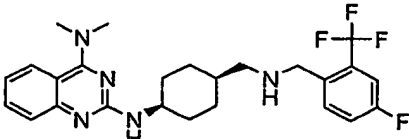
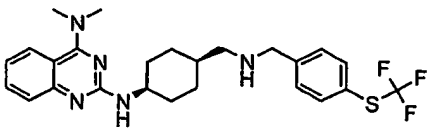
Example No.	Structure	ESI-MS	Retention Time (min)
2891	 $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.00
2892	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.66
2893	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.92
2894	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.71
2895	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.87
2896	 $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.17

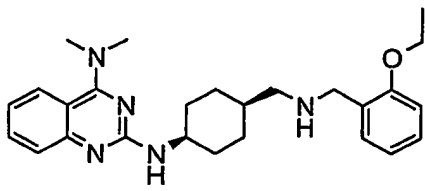
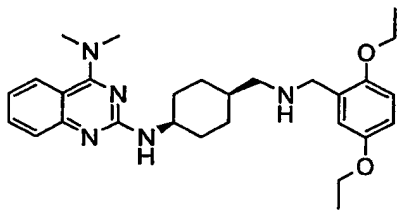
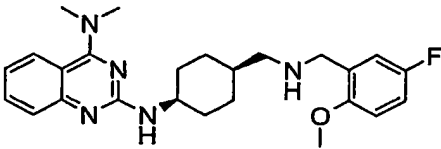
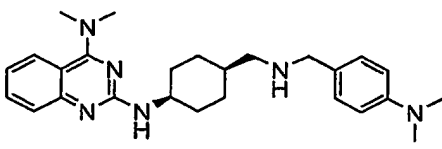
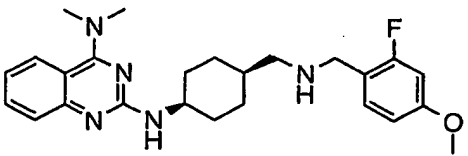
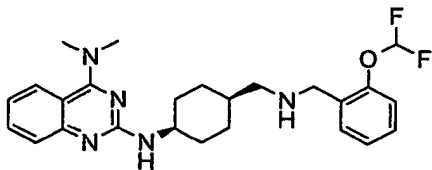
Example No.	Structure	ESI-MS	Retention Time (min)
2897	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)cc(F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.98
2898	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.99
2899	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(Br)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.4 (M + H)	3.15
2900	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.19
2901	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.92
2902	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc5ccccc5c4OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.27

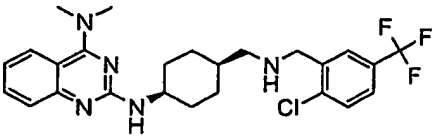
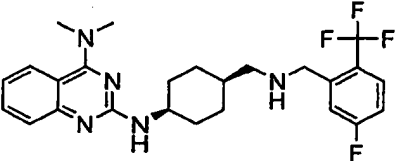
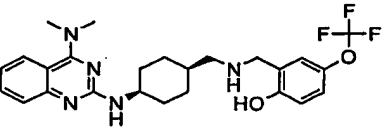
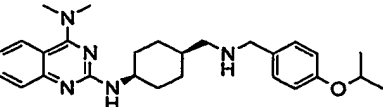
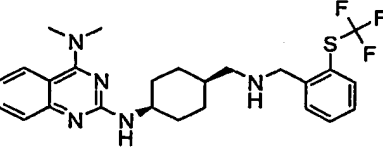
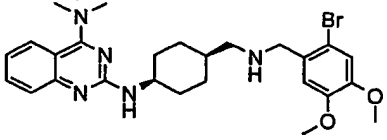
Example No.	Structure	ESI-MS	Retention Time (min)
2903	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.6 (M + H)	2.87
2904	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5c(C)c(C)c(C)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.48
2905	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(C)s5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.96
2906	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(OC)cc(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.03
2907	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(C)c(OC)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.08
2908	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NC4Cc5cc(OC(=O)C)oc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	2.79

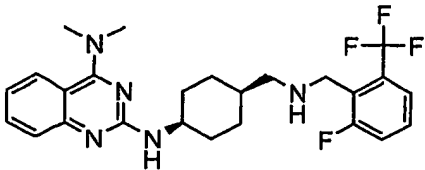
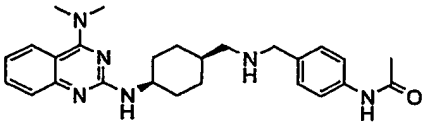
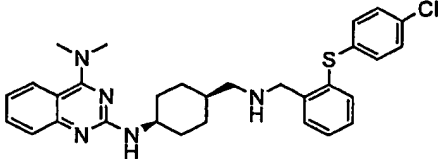
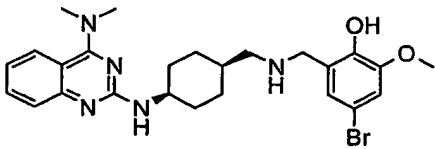
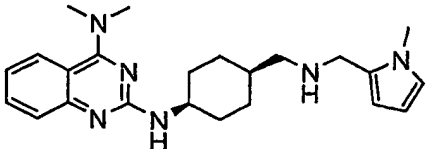
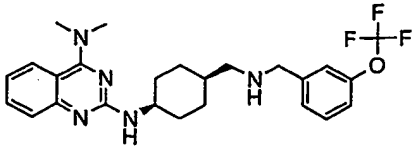
Example No.	Structure	ESI-MS	Retention Time (min)
2909	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.81
2910	 $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	3.21
2911	 $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.08
2912	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.88
2913	 $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.01
2914	 $3\text{CF}_3\text{CO}_2\text{H}$	429.4 (M + H)	2.97

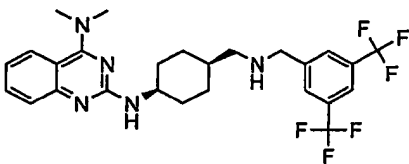
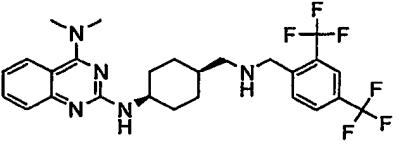
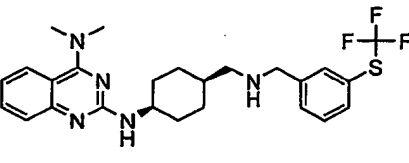
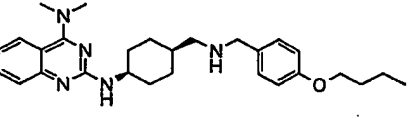
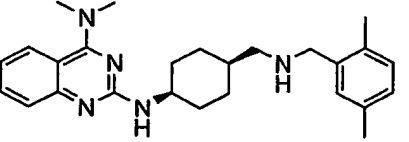
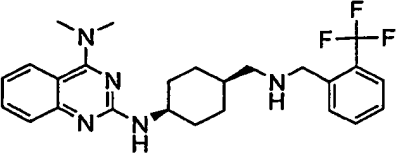
Example No.	Structure	ESI-MS	Retention Time (min)
2915	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.53
2916	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	3.56
2917	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $3\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.80
2918	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.27
2919	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.2 (M + H)	3.10
2920	 <chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C4=CC=CC=C4N3C5=CC=CC=C5N3C6=CC=CC=C6N3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.00

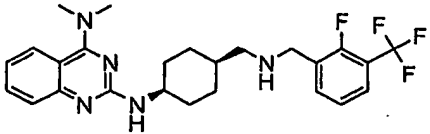
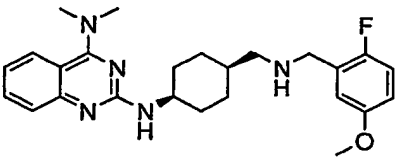
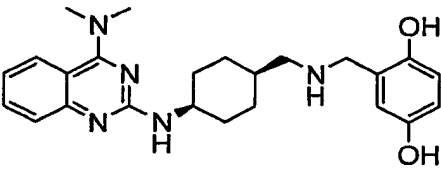
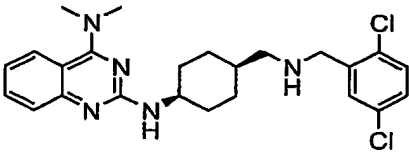
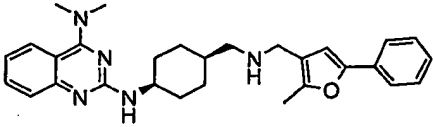
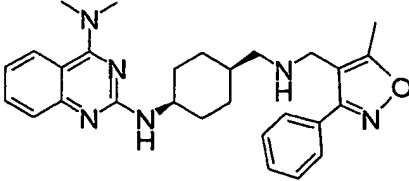
Example No.	Structure	ESI-MS	Retention Time (min)
2921	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(Br)ccc2OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	498.4 (M + H)	3.15
2922	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2c[nH]c3cc(OC)ccc32</chem> $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	2.99
2923	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(F)cc(F)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.0 (M + H)	3.10
2924	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(Cl)cc(O)c2Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	518.2 (M + H)	3.10
2925	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2cc(F)c(F)c(F)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.12
2926	 <chem>CN(C)c1nc2ccccc2n1CN[C@H]1CCCC[C@H]1CNCCc2ccc(SC(F)(F)F)cc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35

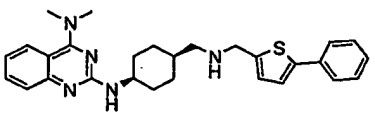
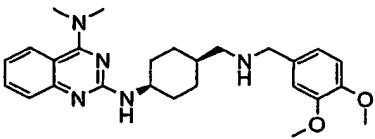
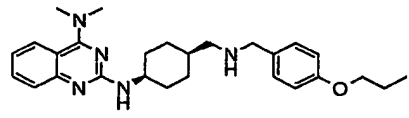
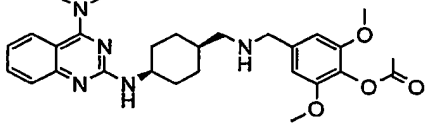
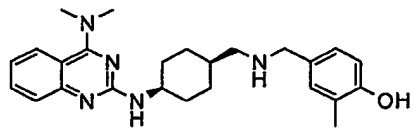
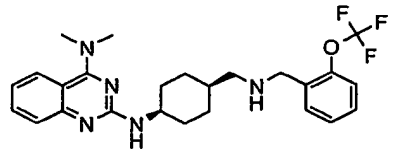
Exemple No.	Structure	ESI-MS	Retention Time (min)
2927	 2CF ₃ CO ₂ H	434.4 (M + H)	3.11
2928	 2CF ₃ CO ₂ H	478.4 (M + H)	3.29
2929	 2CF ₃ CO ₂ H	438.2 (M + H)	3.01
2930	 3CF ₃ CO ₂ H	433.4 (M + H)	2.59
2931	 2CF ₃ CO ₂ H	438.2 (M + H)	2.90
2932	 2CF ₃ CO ₂ H	456.2 (M + H)	3.10

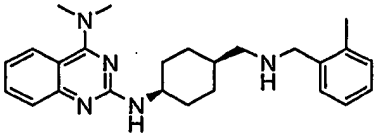
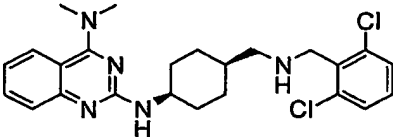
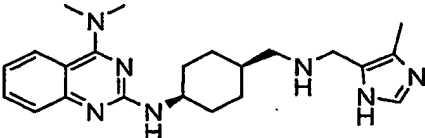
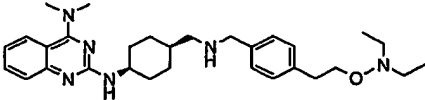
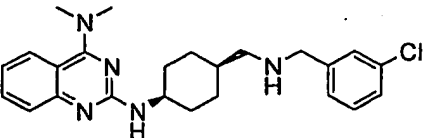
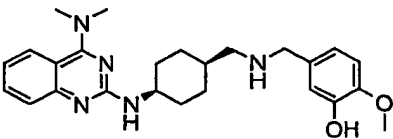
Example No.	Structure	ESI-MS	Retention Time (min)
2933	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(C(F)(F)F)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.25
2934	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.11
2935	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(O)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.20
2936	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(OC(C)C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.17
2937	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(C(F)(F)F)cc4S</chem> $2\text{CF}_3\text{CO}_2\text{H}$	489.6 (M + H)	3.31
2938	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(OC)c(Br)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	3.03

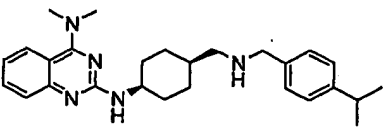
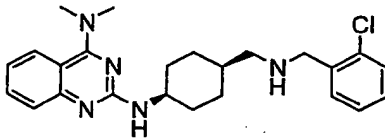
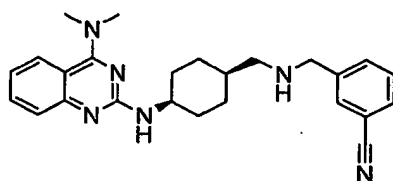
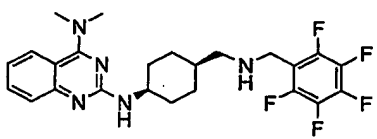
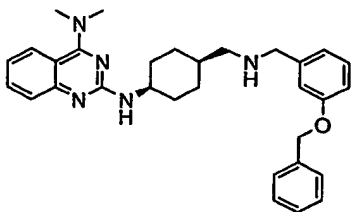
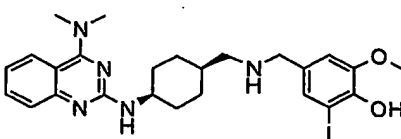
Example No.	Structure	ESI-MS	Retention Time (min)
2939	 $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	2.99
2940	 $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	2.66
2941	 $2\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	3.66
2942	 $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.08
2943	 $3\text{CF}_3\text{CO}_2\text{H}$	393.4 (M + H)	2.79
2944	 $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.24

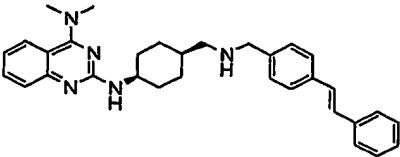
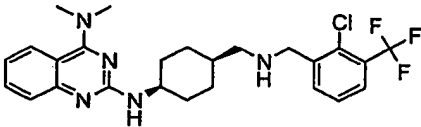
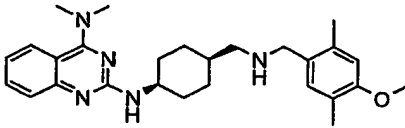
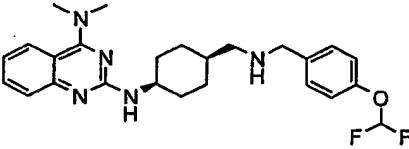
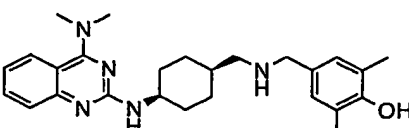
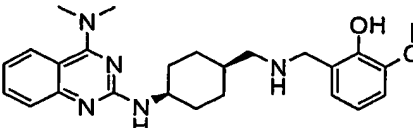
Example No.	Structure	ESI-MS	Retention Time (min)
2945	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4C(F)(F)F)C(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.44
2946	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4C(F)(F)F)C(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.42
2947	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4C(F)(F)F)S(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35
2948	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4)OCC)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.43
2949	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4)C)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.13
2950	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3CNCC4=CC(=CC=C4)C(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.10

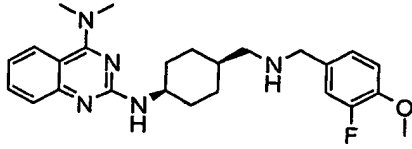
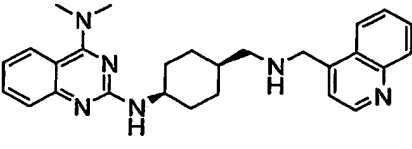
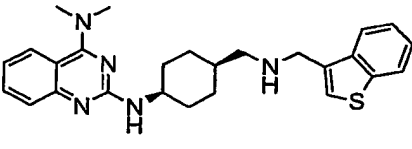
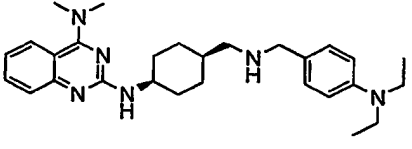
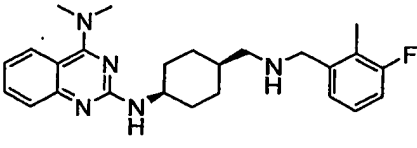
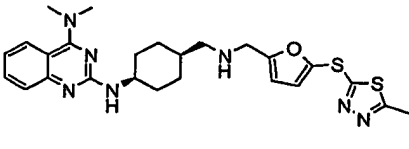
Example No.	Structure	ESI-MS	Retention Time (min)
2951	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4cc(F)c(C(F)(F)F)cc4</chem> $2CF_3CO_2H$	476.4 (M + H)	3.19
2952	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4cc(F)cc(OC)c4</chem> $2CF_3CO_2H$	438.2 (M + H)	2.95
2953	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4cc(O)cc(O)c4</chem> $2CF_3CO_2H$	422.4 (M + H)	2.61
2954	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4cc(Cl)cc(Cl)c4</chem> $2CF_3CO_2H$	458.2 (M + H)	3.07
2955	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4oc(Cc5ccccc5)c4</chem> $2CF_3CO_2H$	470.4 (M + H)	3.45
2956	 <chem>CN(C)c1nc2ccccc2n1N[C@H]3CCCC[C@H]3CNCCc4c5ccccc5n4OC</chem> $2CF_3CO_2H$	471.6 (M + H)	2.88

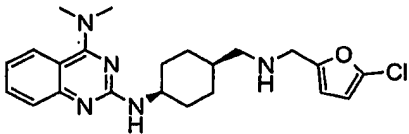
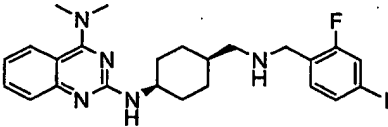
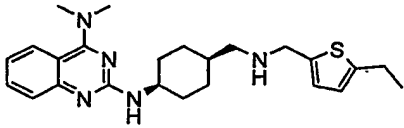
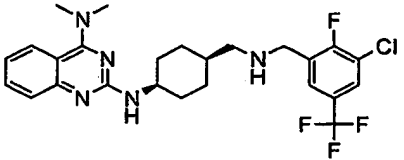
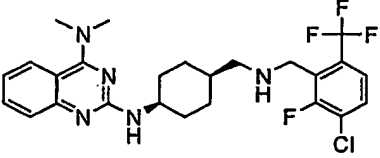
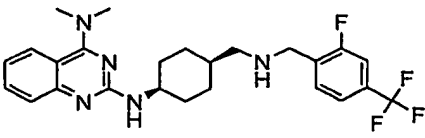
Example No.	Structure	ESI-MS	Retention Time (min)
2957	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=C5C(=C4)SC(=C5)c6ccccc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.36
2958	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC(OC)=CC(OC)=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450 (M + H)	2.75
2959	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=CC(=C4)OCC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.20
2960	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC(OC)=CC(=C4)C(=O)OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	508.4 (M + H)	3.00
2961	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC(=C(C)C)C(=C4)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.80
2962	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCC4=CC=C(C=C4)OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.20

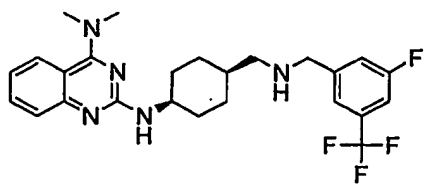
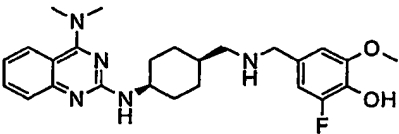
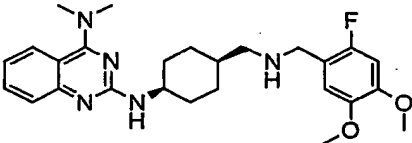
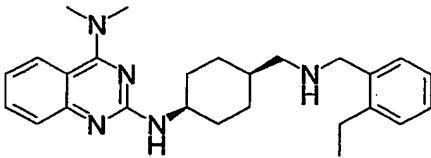
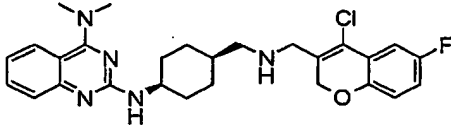
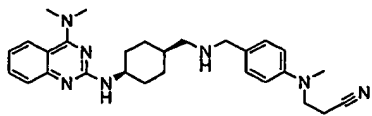
Example No.	Structure	ESI-MS	Retention Time (min)
2963	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(C)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	2.87
2964	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(Cl)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.00
2965	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4c[nH]c5c4C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.30
2966	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(COCCN)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	505.4 (M + H)	2.60
2967	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.00
2968	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(OC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.71

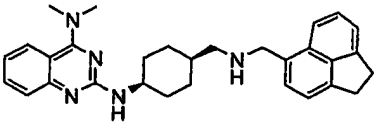
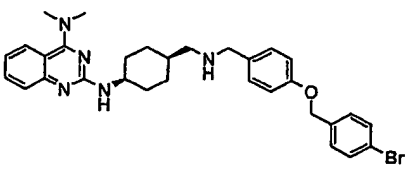
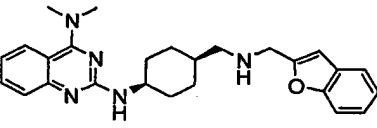
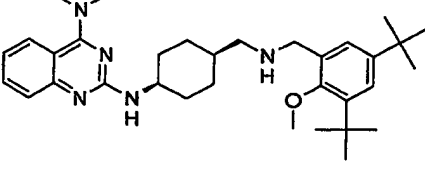
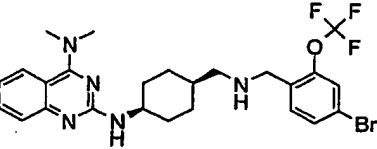
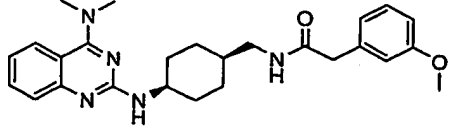
Example No.	Structure	ESI-MS	Retention Time (min)
2969	 <chem>CC(C)c1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.30
2970	 <chem>Clc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.95
2971	 <chem>N#Cc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.79
2972	 <chem>Fc1cc(F)c(F)c(F)c1CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.00
2973	 <chem>c1ccc(cc1)Oc2ccc(cc2)CNCC3CCCCC3Nc4nc5ccccc5n4C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.2 (M + H)	3.46
2974	 <chem>COc1cc(I)ccc1CNCC2CCCCC2Nc3nc4ccccc4n3C(C)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	2.99

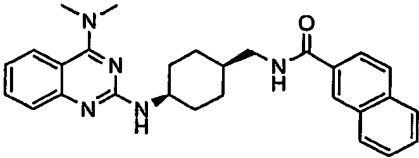
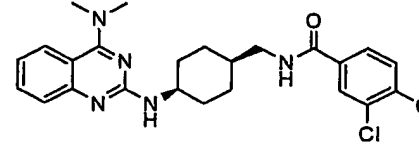
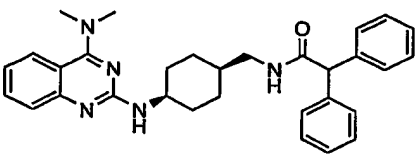
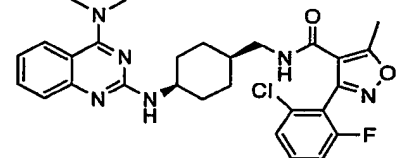
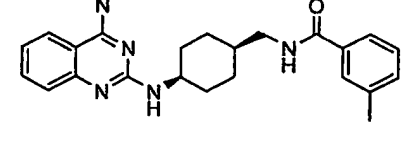
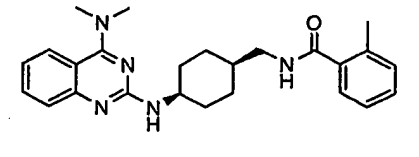
Example No.	Structure	ESI-MS	Retention Time (min)
2975	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=CC=C4/C=C/C5=CC=CC=C5)c3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.4 (M + H)	3.64
2976	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)Cl)C(F)(F)F)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.25
2977	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)OC)C)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.22
2978	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)C(F)F)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	3.09
2979	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)O)C)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.89
2980	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)OC)O)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.79

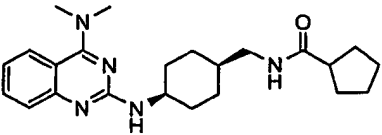
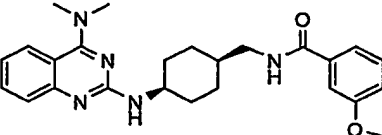
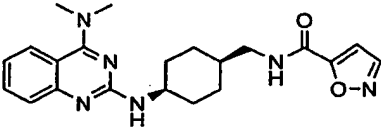
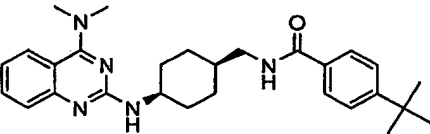
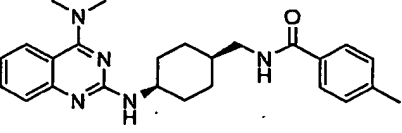
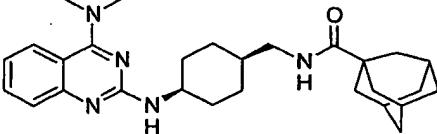
Example No.	Structure	ESI-MS	Retention Time (min)
2981	 $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.91
2982	 $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.55
2983	 $2\text{CF}_3\text{CO}_2\text{H}$	446.4 (M + H)	3.13
2984	 $3\text{CF}_3\text{CO}_2\text{H}$	461.4 (M + H)	2.46
2985	 $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.01
2986	 $2\text{CF}_3\text{CO}_2\text{H}$	510.2 (M + H)	2.85

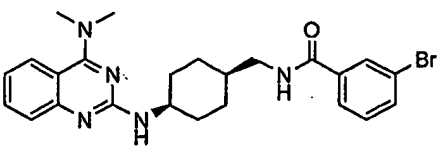
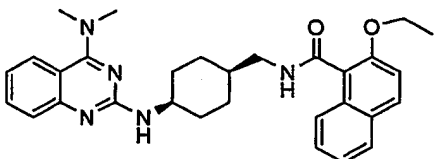
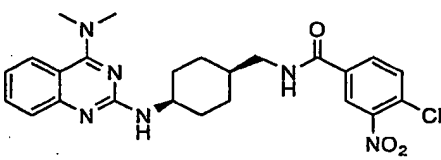
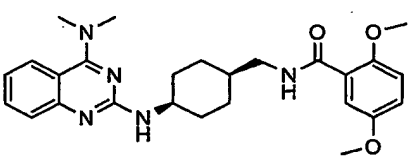
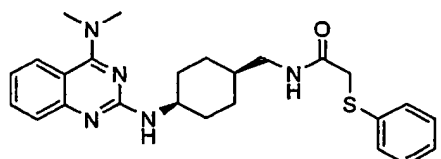
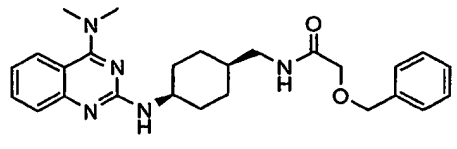
Example No.	Structure	ESI-MS	Retention Time (min)
2987	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC(=C(C=C4)O)C=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	414.4 (M + H)	2.86
2988	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC(=C(C=C4)F)C=C4I</chem> $2\text{CF}_3\text{CO}_2\text{H}$	534.2 (M + H)	3.13
2989	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC=C(C=C4)S</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.08
2990	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC(=C(C=C4)F)C=C4C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.32
2991	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC(=C(C=C4)F)C=C4C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
2992	 <chem>CC1=NC2=CC=CC=C2N1NC3CCCCC3CNCC4=CC(=C(C=C4)F)C=C4C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.17

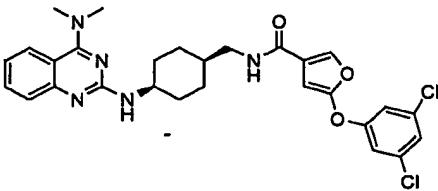
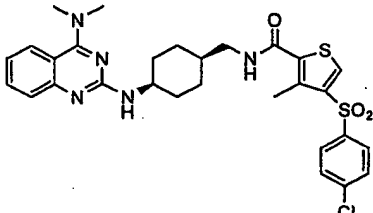
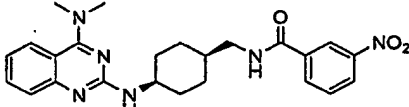
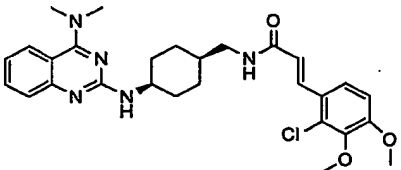
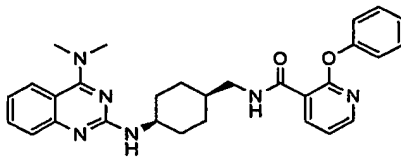
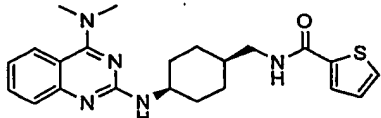
Example No.	Structure	ESI-MS	Retention Time (min)
2993	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(F)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.21
2994	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(OC)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.77
2995	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4cc(OC)c(F)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.89
2996	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4ccccc4CC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.12
2997	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4c5cc(F)ccc5oc4Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
2998	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNCCc4ccc(NC(C)C)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	2.99

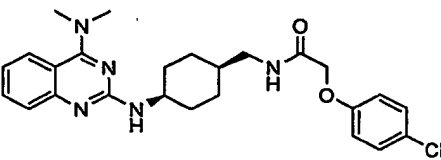
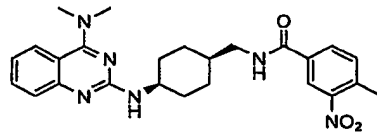
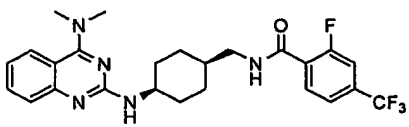
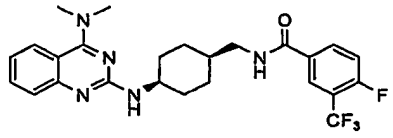
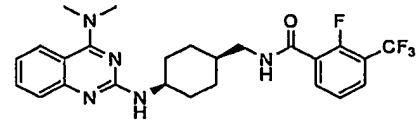
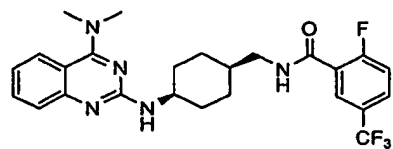
Example No.	Structure	ESI-MS	Retention Time (min)
2999	 <chem>2CF3CO2H</chem>	466.4 (M + H)	3.37
3000	 <chem>2CF3CO2H</chem>	574.2 (M + H)	3.64
3001	 <chem>2CF3CO2H</chem>	430.4 (M + H)	3.05
3002	 <chem>2CF3CO2H</chem>	532.4 (M + H)	4.05
3003	 <chem>2CF3CO2H</chem>	552.0 (M + H)	3.37
3004	 <chem>CF3CO2H</chem>	448.4 (M + H)	3.51

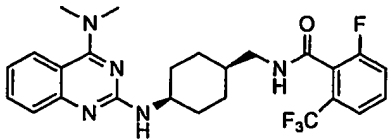
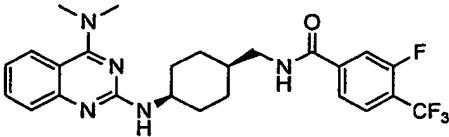
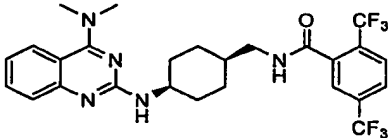
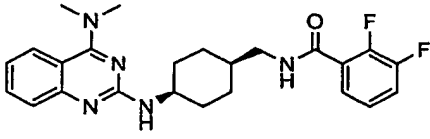
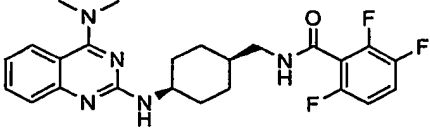
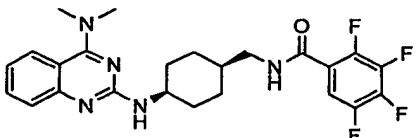
Example No.	Structure	ESI-MS	Retention Time (min)
3005	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)c4ccc5ccccc45</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.91
3006	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.02
3007	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)C(c1ccccc1)c2ccccc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	4.01
3008	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)Nc4c(Cl)c(F)c5nnoc54</chem> $\text{CF}_3\text{CO}_2\text{H}$	537.4 (M + H)	3.77
3009	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.63
3010	 <chem>CC1=CN=C2C(=N1)N=CN=C2C3CCCCC3CCNC(=O)c4cc(C)cccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.51

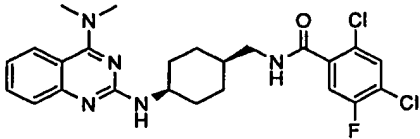
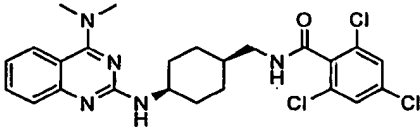
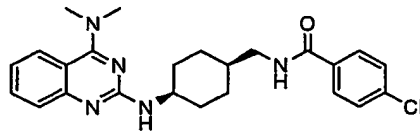
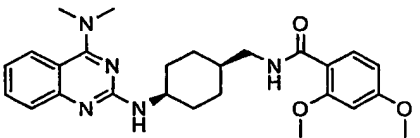
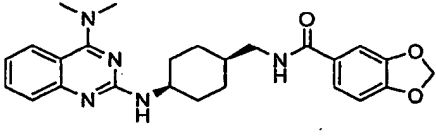
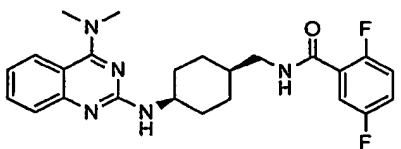
Example No.	Structure	ESI-MS	Retention Time (min)
3011	 <chem>CC1=NC2=CC=CC=C2N=C(N[C@H]3CCCC[C@H]3CNC(=O)C4CCCC4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	3.47
3012	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2CNC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.52
3013	 <chem>Cc1ccoc1C(=O)N[C@H]2CCCC[C@H]2CNC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	395.4 (M + H)	3.15
3014	 <chem>CC(C)(C)c1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2CNC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	4.03
3015	 <chem>Cc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2CNC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.65
3016	 <chem>C1=CC=C2C(=C1)N3=CC=CC=C3N(C)C2=NC4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.09

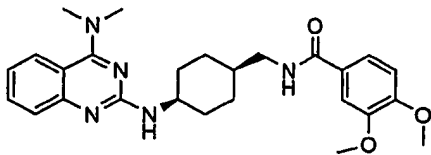
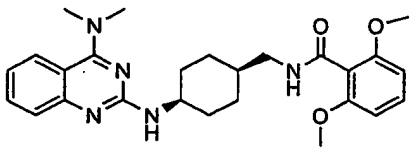
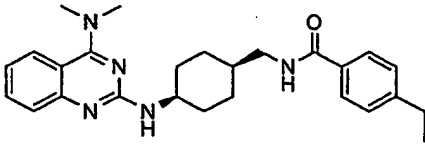
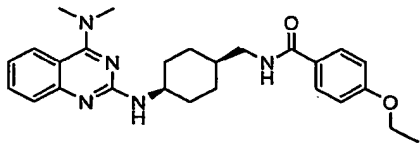
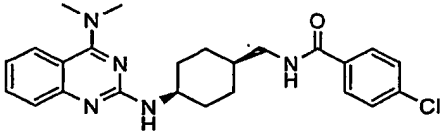
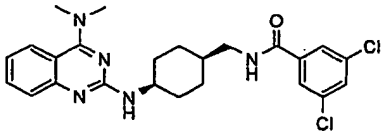
Example No.	Structure	ESI-MS	Retention Time (min)
3017	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(Br)cc4)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	3.79
3018	 <chem>CCOC(=O)N[C@H]1CCCC[C@H]1Nc2nc3c(ncn3C2N(C)C)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.6 (M + H)	3.88
3019	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)c4cc([N+](=O)[O-])ccc4Cl)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	3.80
3020	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)c4cc(OC)cc4OC)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.49
3021	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)Sc4ccccc4)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.61
3022	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NC(=O)OCCc4ccccc4)[C+]([N-])</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.2 (M + H)	3.70

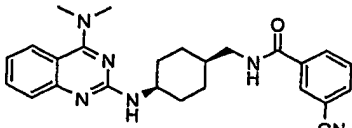
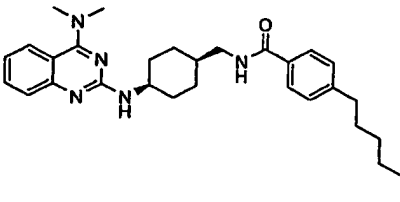
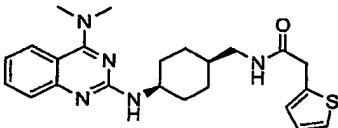
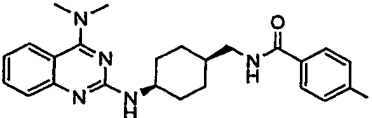
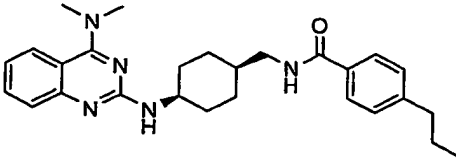
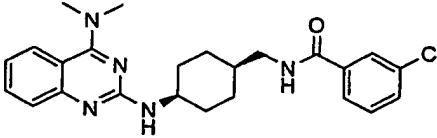
Example No.	Structure	ESI-MS	Retention Time (min)
3023	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Oc5cc(Cl)cc(Cl)c5)oc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	554.4 (M + H)	4.41
3024	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c4sc(S(=O)(=O)c5ccc(Cl)cc5)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	4.03
3025	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c4ccc([N+](=O)[O-])cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	499.2 (M + H)	3.59
3026	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)/C=C/c4cc(OC)c(OC)c(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.84
3027	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c4ccncc4Oc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	3.80
3028	 <chem>CC1=NC2=CC=CC=C2N1C(C)N[C@H]3CCCC[C@H]3CNC(=O)c4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.43

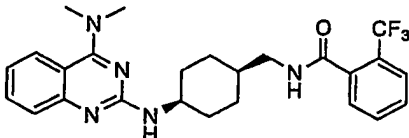
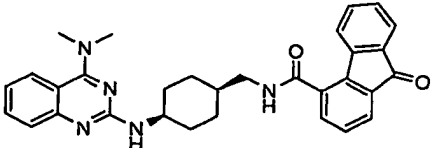
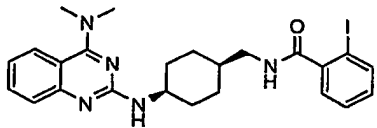
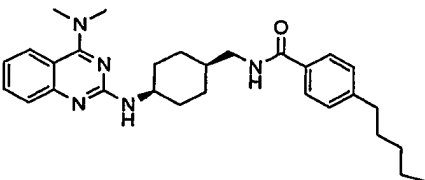
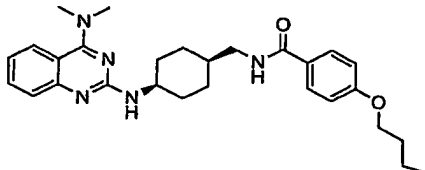
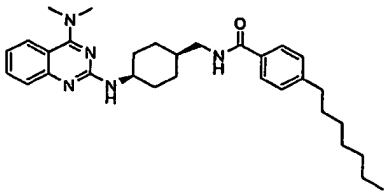
Example No.	Structure	ESI-MS	Retention Time (min)
3029	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)COC4=CC=C(C=C4)Cl)N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.77
3030	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)[N+](=O)[O-])N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	463.2 (M + H)	3.73
3031	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)F(C)F(C)F)N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.91
3032	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)F(C)F(C)F)N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.94
3033	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)F(C)F(C)F)N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.85
3034	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3CNC(=O)C4=CC(=CC=C4)F(C)F(C)F)N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.87

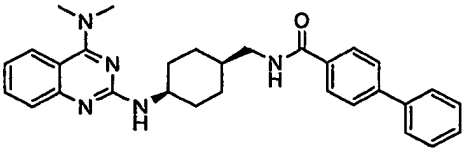
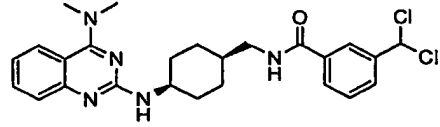
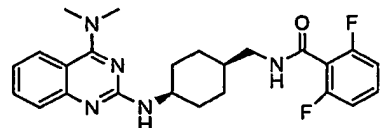
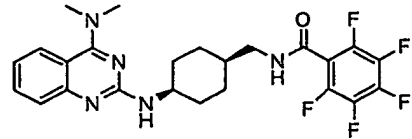
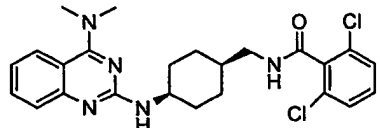
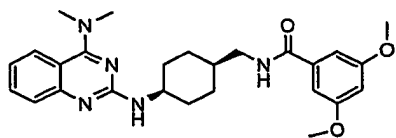
Example No.	Structure	ESI-MS	Retention Time (min)
3035	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.63
3036	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.54
3037	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	3.95
3038	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)cc(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.58
3039	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.56
3040	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(F)c(F)c4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.83

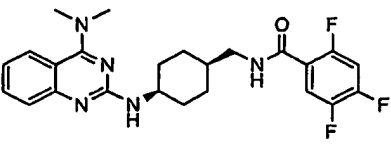
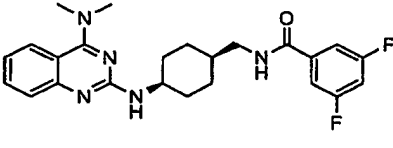
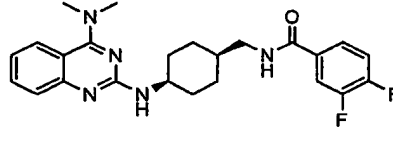
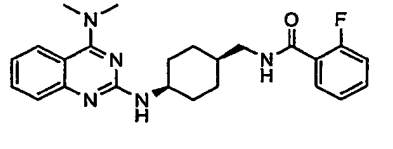
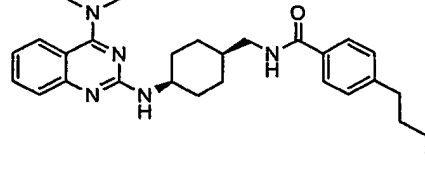
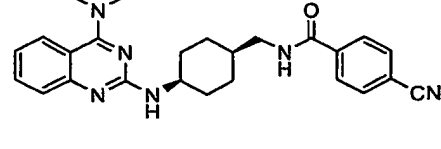
Example No.	Structure	ESI-MS	Retention Time (min)
3041	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Cl)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.82
3042	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Cl)c(Cl)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.0 (M + H)	3.85
3043	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4cccc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.71
3044	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(OC)cc(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.65
3045	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4ccc5c(c4)OCO5</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.47
3046	 <chem>CC1=CN2C(=N1)N(C2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.59

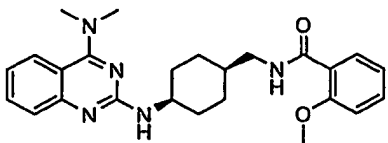
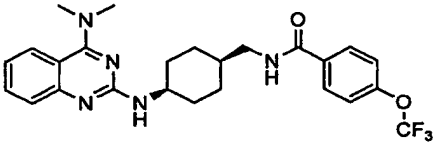
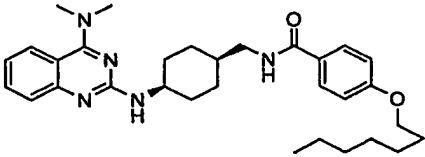
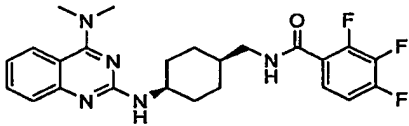
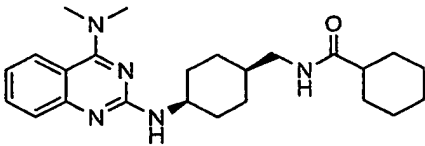
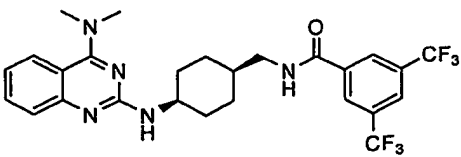
Example No.	Structure	ESI-MS	Retention Time (min)
3047	 <chem>COc1cc(OC)c(OC)c(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.36
3048	 <chem>COc1cc(OC)c(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)c(O)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.39
3049	 <chem>CCc1ccc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.81
3050	 <chem>CCOC1=CC=C(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.69
3051	 <chem>Clc1ccc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.69
3052	 <chem>Clc1cc(C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C)cc(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.03

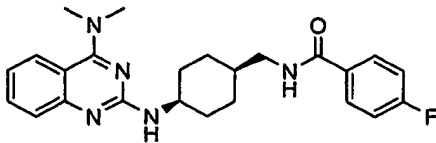
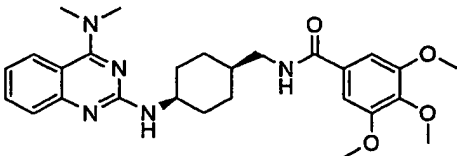
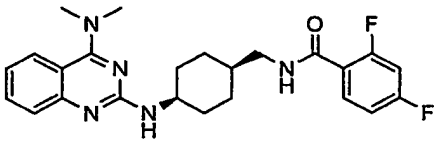
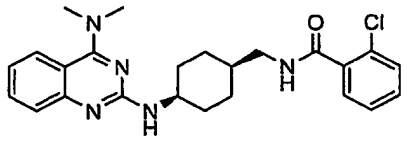
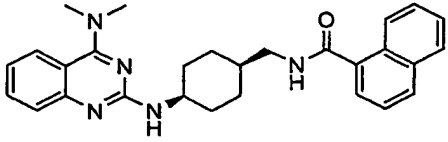
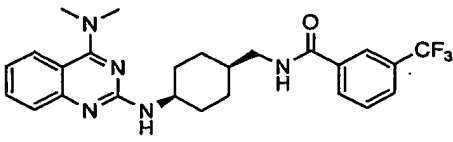
Example No.	Structure	ESI-MS	Retention Time (min)
3053	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C#N)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	429.2 (M + H)	3.47
3054	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(CCCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	4.60
3055	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)Cc4ccsc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.41
3056	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(I)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	3.83
3057	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(CCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.4 (M + H)	4.02
3058	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.70

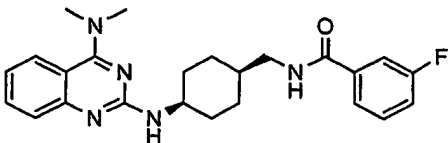
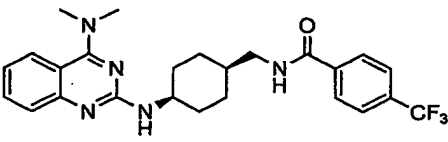
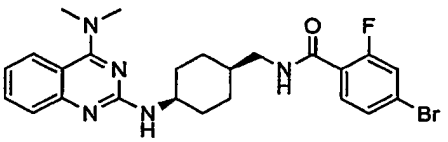
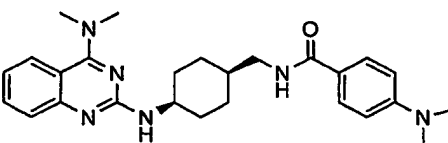
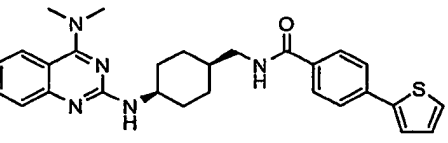
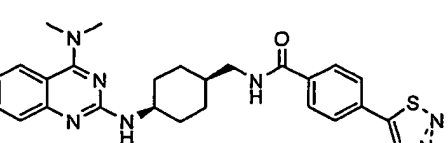
Example No.	Structure	ESI-MS	Retention Time (min)
3059	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.55
3060	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.71
3061	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.2 (M + H)	3.61
3062	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.41
3063	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.14
3064	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.4 (M + H)	4.83

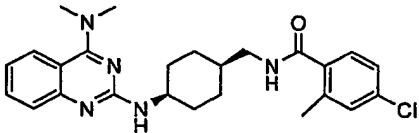
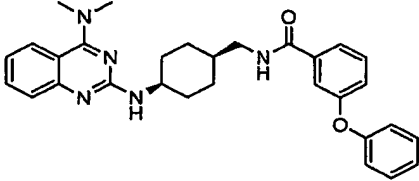
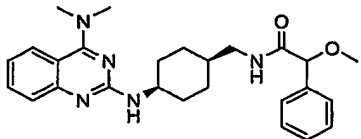
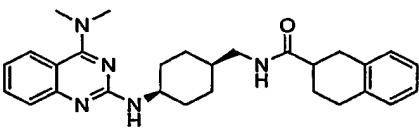
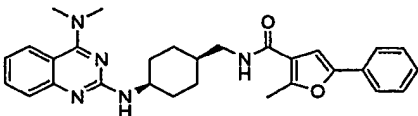
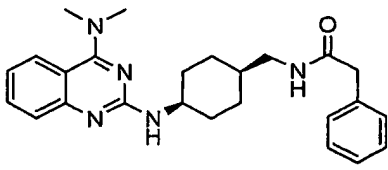
Example No.	Structure	ESI-MS	Retention Time (min)
3065	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(cc4)-c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.09
3066	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(cc4)C(Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.4 (M + H)	3.84
3067	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)ccc4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.46
3068	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4c(F)c(F)c(F)c4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.79
3069	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Cl)ccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.55
3070	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3CNC(=O)c4cc(OC)cc(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.63

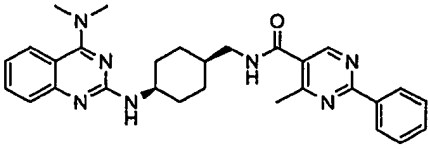
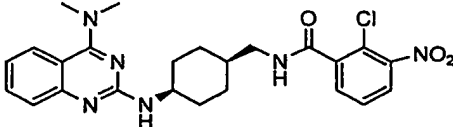
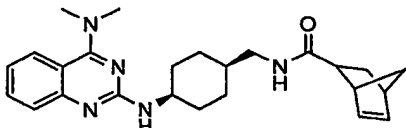
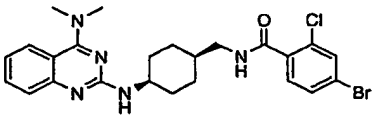
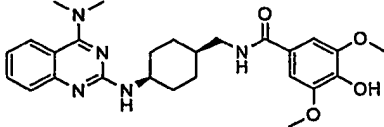
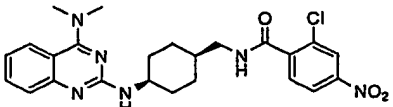
Example No.	Structure	ESI-MS	Retention Time (min)
3071	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5cc(F)c(F)c(F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.69
3072	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5cc(F)c(F)c(F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.69
3073	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5cc(F)c(F)c(F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.66
3074	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5ccccc5F</chem> $\text{CF}_3\text{CO}_2\text{H}$	422.4 (M + H)	3.55
3075	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5ccc(CCC)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	4.24
3076	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CCNC(=O)c5ccc(C#N)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	429.2 (M + H)	3.42

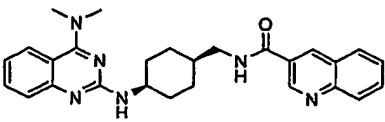
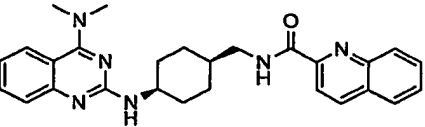
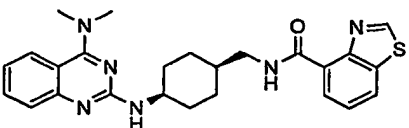
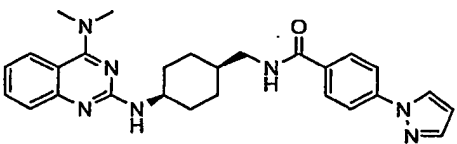
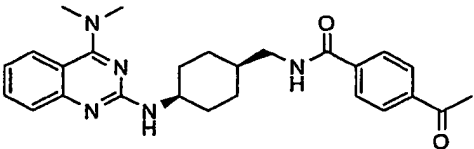
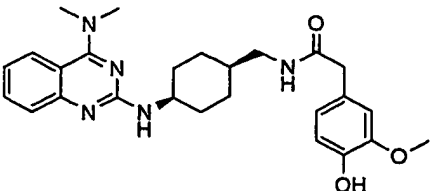
Example No.	Structure	ESI-MS	Retention Time (min)
3077	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.61
3078	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.86
3079	 <chem>CCCCCOc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.74
3080	 <chem>Fc1cc(F)c(F)cc1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.68
3081	 <chem>C1CCCCC1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.58
3082	 <chem>Cc1cc(C)cc(C(F)(F)F)c1C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	4.19

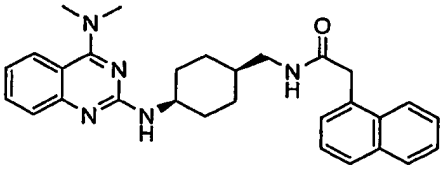
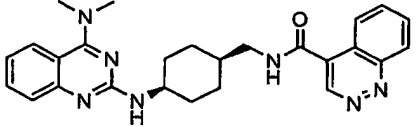
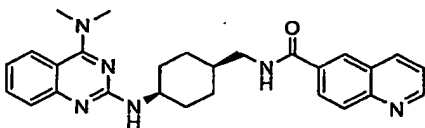
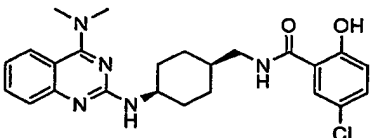
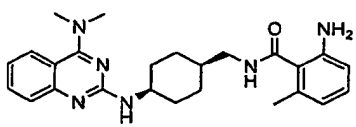
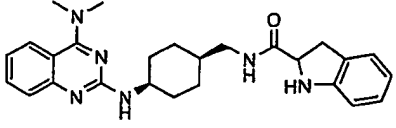
Example No.	Structure	ESI-MS	Retention Time (min)
3083	 <chem>CC1=NC2=CC=CC=C2N(C)N1[C@H]3CCCC[C@H]3CNC(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.50
3084	 <chem>COc1cc(OC)c(OC)c(C(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3C=C1)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.39
3085	 <chem>Fc1cc(C(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3C=C1)c(F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.55
3086	 <chem>Clc1ccccc1C(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.48
3087	 <chem>c1ccc2cc(C(=O)N[C@H]3CCCC[C@H]3C4=NC5=CC=CC=C5N(C)N4=C2C=C1)ccc2ccccc12</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.75
3088	 <chem>Cc1ccc(C(=O)N[C@H]2CCCC[C@H]2C3=NC4=CC=CC=C4N(C)N3C=C1)cc1C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.83

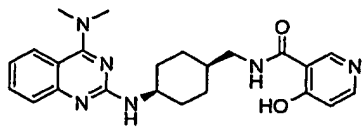
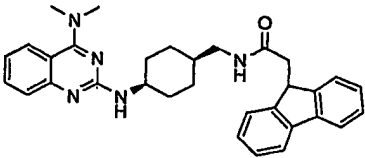
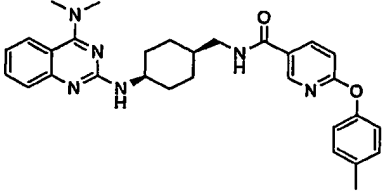
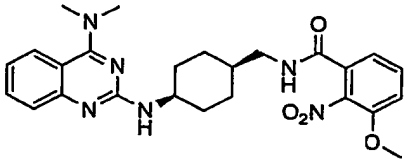
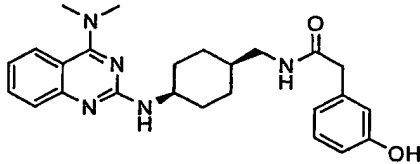
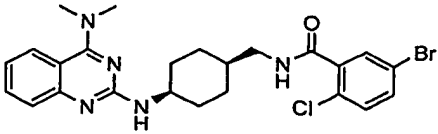
Example No.	Structure	ESI-MS	Retention Time (min)
3089	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.51
3090	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4ccc(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.87
3091	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4cc(F)cc(Br)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.4 (M + H)	3.03
3092	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4ccc(N(C)C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	2.59
3093	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4ccc(c4)c5ccsc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.4 (M + H)	3.25
3094	 <chem>CC1=NC2=CC=CC=C2N(C)=N1[C@H]3CCCC[C@@H]3NC(=O)c4ccc(c4)c5nn[nH]5</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	2.81

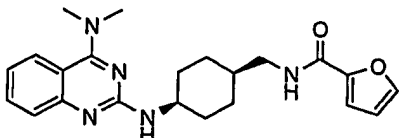
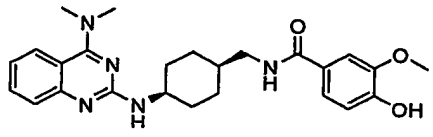
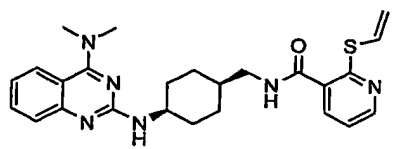
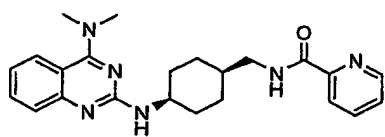
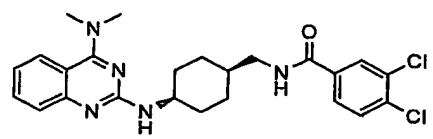
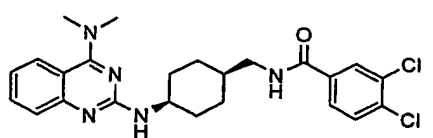
Example No.	Structure	ESI-MS	Retention Time (min)
3095	 <chem>CC1=CC=C(C=C1C(=O)NCC2=CC=CC=C2N2C(C)=NC3=CC=CC=C3N2C)C4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	452.4 (M + H)	2.98
3096	 <chem>COc1ccc(cc1C(=O)NCC2=CC=CC=C2N2C(C)=NC3=CC=CC=C3N2C)C4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
3097	 <chem>COC(=O)C1=CC=CC=C1C(=O)NCC2=CC=CC=C2N2C(C)=NC3=CC=CC=C3N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.77
3098	 <chem>O=C1C2=CC=CC=C2CCC1C(=O)NCC3=CC=CC=C3N3C(C)=NC4=CC=CC=C4N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.06
3099	 <chem>O=C1C2=CC=CC=C2C(=O)N1C(=O)NCC3=CC=CC=C3N3C(C)=NC4=CC=CC=C4N3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	3.40
3100	 <chem>CC(=O)C1=CC=CC=C1C(=O)NCC2=CC=CC=C2N2C(C)=NC3=CC=CC=C3N2C</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	2.69

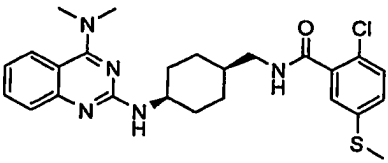
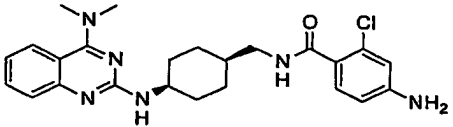
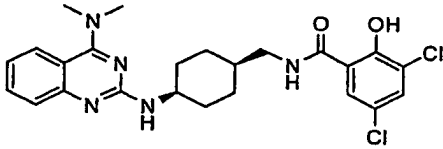
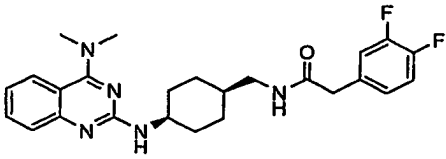
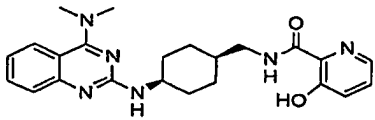
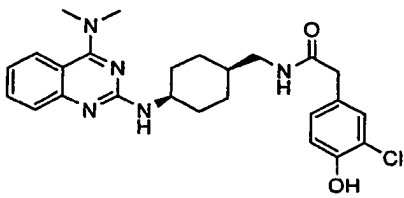
Example No.	Structure	ESI-MS	Retention Time (min)
3101	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CN(C)C(=O)N=C4C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.01
3102	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC(=CC=C4)C(=O)N=C4C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	2.79
3103	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC5C(C4)C=CC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.76
3104	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC(=CC=C4)C(=O)N=C4C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	3.03
3105	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC(=CC=C4)C(=O)N=C4C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.41
3106	 <chem>CC1=CN2C(=N1)C(=N2)C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC(=CC=C4)C(=O)N=C4C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.84

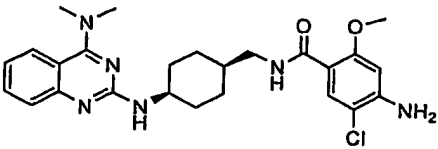
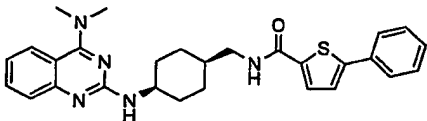
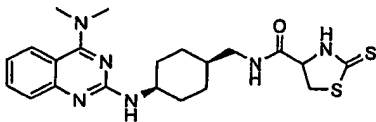
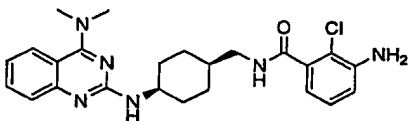
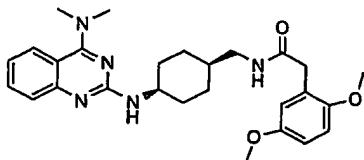
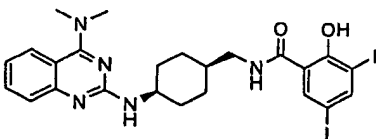
Example No.	Structure	ESI-MS	Retention Time (min)
3107	 $2\text{CF}_3\text{CO}_2\text{H}$	455 (M + H)	2.45
3108	 $2\text{CF}_3\text{CO}_2\text{H}$	455.2 (M + H)	3.19
3109	 $\text{CF}_3\text{CO}_2\text{H}$	461.4 (M + H)	2.60
3110	 $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	2.74
3111	 $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	2.61
3112	 $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.35

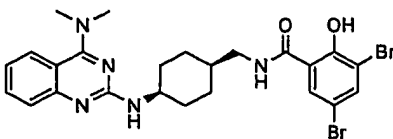
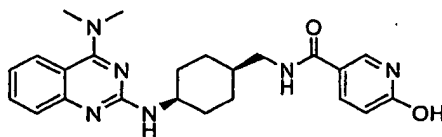
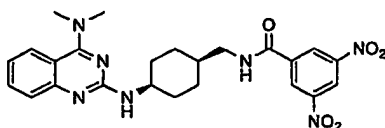
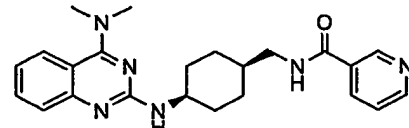
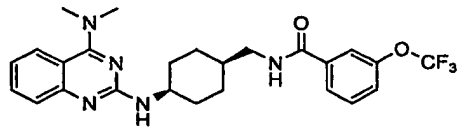
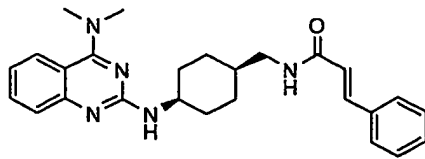
Example No.	Structure	ESI-MS	Retention Time (min)
3113	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6ccccc6)N1C</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.04
3114	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6ccncc6)N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	2.44
3115	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6ccc7ccncc7c6)N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	455.2 (M + H)	2.11
3116	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6cc(Cl)ccc6O)N1C</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.21
3117	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6cc(C)c(N)cc6)N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	433.6 (M + H)	2.34
3118	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3Cc4nc5ccccc5cc4C(=O)Nc6c[nH]c7ccccc67)N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	444.6 (M+)	2.93

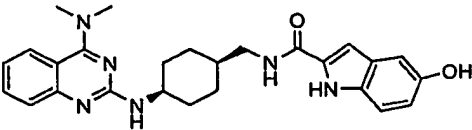
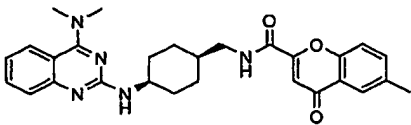
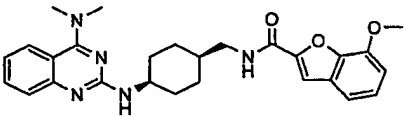
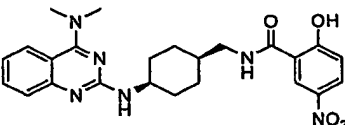
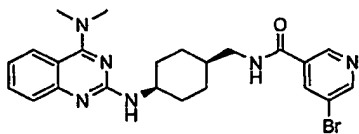
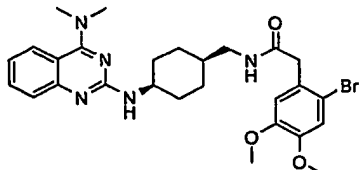
Example No.	Structure	ESI-MS	Retention Time (min)
3119	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4ccncc4O</chem> <chem>2CF3CO2H</chem>	421.4 (M + H)	2.23
3120	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)CCc4c5ccccc5c6ccccc46</chem> <chem>CF3CO2H</chem>	506.4 (M + H)	3.31
3121	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4cc(OC)ncn4</chem> <chem>2CF3CO2H</chem>	511.6 (M + H)	3.21
3122	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4cc(OC)cc([N+](=O)[O-])c4</chem> <chem>CF3CO2H</chem>	479.4 (M + H)	3.60
3123	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)Cc1cccc(O)c1</chem> <chem>CF3CO2H</chem>	434.4 (M + H)	2.37
3124	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c1cc(Br)ccc1Cl</chem> <chem>CF3CO2H</chem>	516.4 (M + H)	3.02

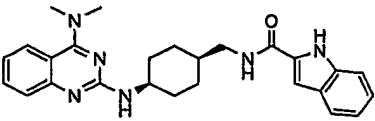
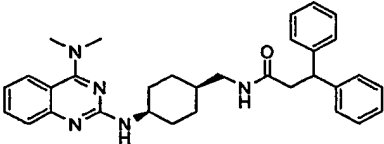
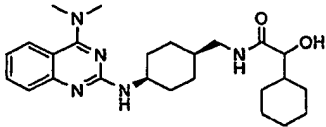
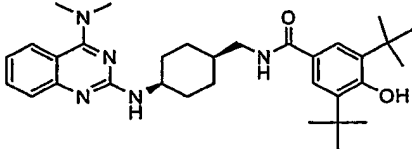
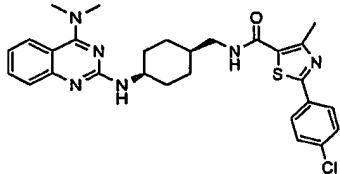
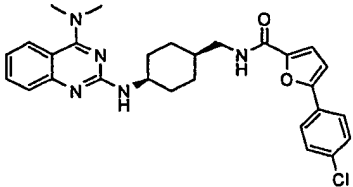
Example No.	Structure	ESI-MS	Retention Time (min)
3125	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CN(C(=O)Oc1ccoc1)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.45
3126	 <chem>COc1cccc(c1)C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3c1ccccc1nnc3N(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.2 (M + H)	2.41
3127	 <chem>C=CS1=CC=CC=C1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3c1ccccc1nnc3N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.0 (M + H)	2.88
3128	 <chem>c1cccnc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3c1ccccc1nnc3N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	2.61
3129	 <chem>Clc1cc(Cl)ccc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3c1ccccc1nnc3N(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	3.17
3130	 <chem>Clc1cc(Cl)ccc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3c1ccccc1nnc3N(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.59

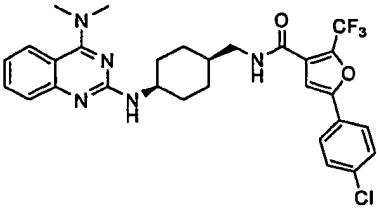
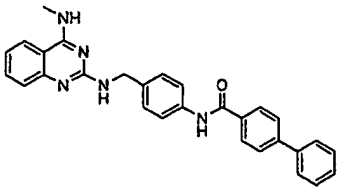
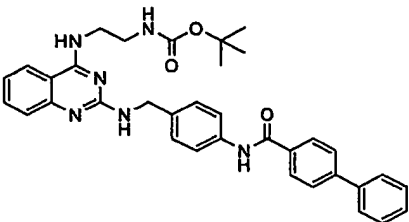
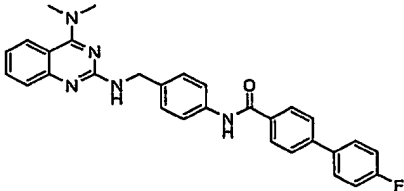
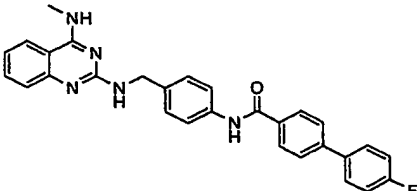
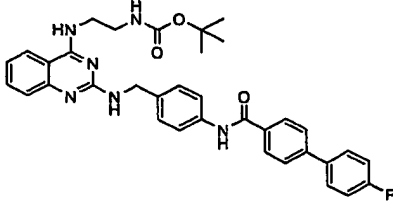
Example No.	Structure	ESI-MS	Retention Time (min)
3131	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)S</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	2.99
3132	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	453.0 (M + H)	2.45
3133	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.59
3134	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.81
3135	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	421.4 (M + H)	2.89
3136	 <chem>CC1=CC=C2N=CN(C)C2=C1C3=CC=C(C=C3)NC4=CC=C(C=C4)C(=O)N5C=CC(=C5)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.53

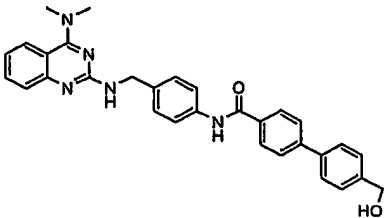
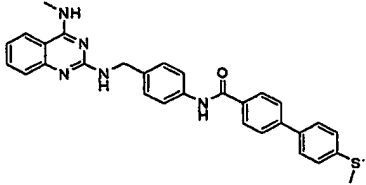
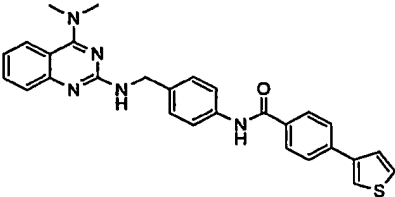
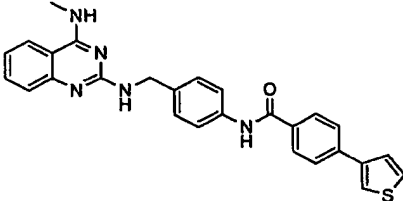
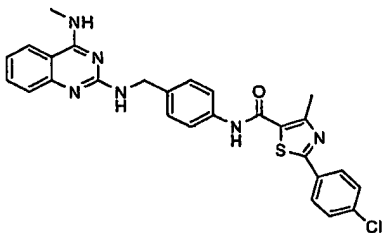
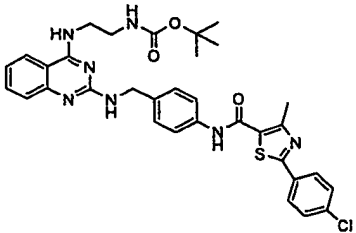
Example No.	Structure	ESI-MS	Retention Time (min)
3137	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=C(C=C4)C(=O)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.83
3138	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=C(C=C4)S5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	487.4 (M+2H+)	3.40
3139	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=CC=C4S5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	445.6 (M + H)	2.36
3140	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=C(C=C4)C(=O)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	453.2 (M + H)	2.46
3141	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=C(C=C4)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.77
3142	 <chem>CN1C=NC2=C(N1)C=CC=C2C3=CC=CC=C3N3CCCCC3CCNC(=O)C4=CC=C(C=C4)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	672.2 (M + H)	3.92

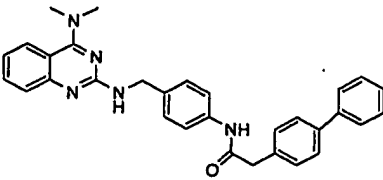
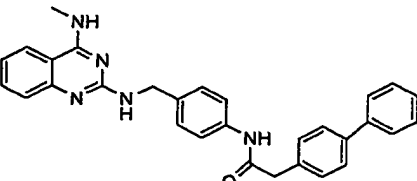
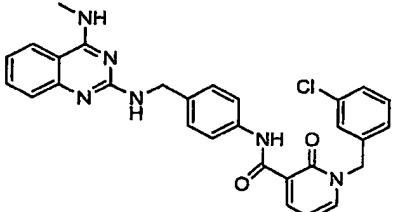
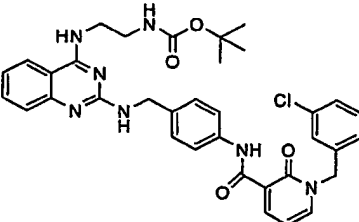
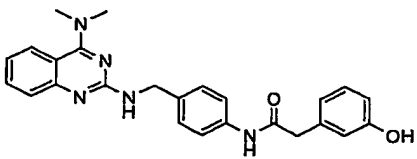
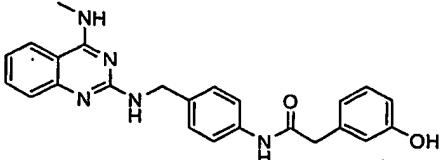
Example No.	Structure	ESI-MS	Retention Time (min)
3143	 $\text{CF}_3\text{CO}_2\text{H}$	576.2 (M + H)	3.71
3144	 $2\text{CF}_3\text{CO}_2\text{H}$	421.2 (M + H)	2.01
3145	 $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.77
3146	 $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	1.99
3147	 $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.13
3148	 $\text{CF}_3\text{CO}_2\text{H}$	430.4 (M + H)	2.91

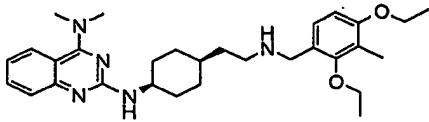
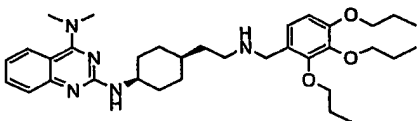
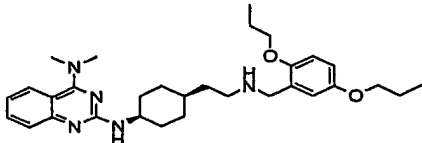
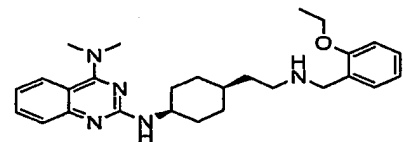
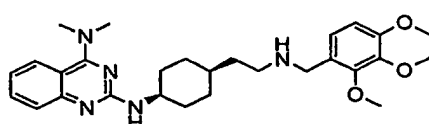
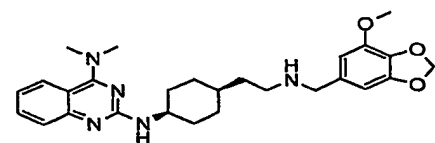
Example No.	Structure	ESI-MS	Retention Time (min)
3149	 <p>2CF₃CO₂H</p>	459.4 (M + H)	2.47
3150	 <p>CF₃CO₂H</p>	486.6 (M + H)	2.93
3151	 <p>CF₃CO₂H</p>	474.4 (M + H)	3.03
3152	 <p>CF₃CO₂H</p>	465.2 (M + H)	3.13
3153	 <p>2CF₃CO₂H</p>	483.4 (M + H)	2.67
3154	 <p>CF₃CO₂H</p>	556.4 (M + H)	2.84

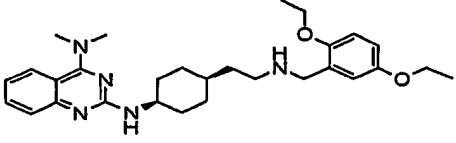
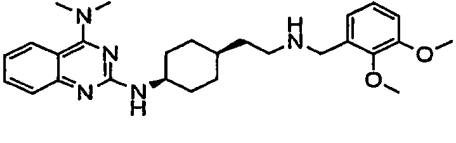
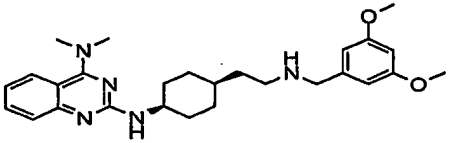
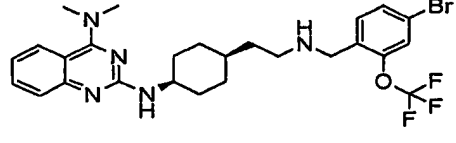
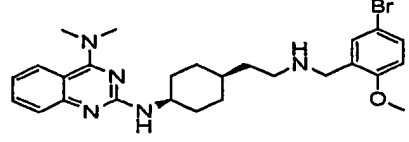
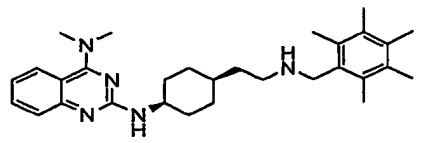
Example No.	Structure	ESI-MS	Retention Time (min)
3155	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4c[nH]c5ccccc45</chem> $2CF_3CO_2H$	443.4 (M + H)	2.94
3156	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)CC(c1ccccc1)c2ccccc2</chem> CF_3CO_2H	508.2 (M + H)	3.20
3157	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)CC4CCCCC4C(=O)O</chem> CF_3CO_2H	440.0 (M + H)	2.72
3158	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4c(O)c(C)(C)c(C)c4</chem> CF_3CO_2H	532.4 (M + H)	3.58
3159	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4nc(C)s(c4)c5ccc(Cl)cc5</chem> CF_3CO_2H	535.4 (M + H)	3.51
3160	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3CCCCC3CCNC(=O)c4oc(C)c(c4)c5ccc(Cl)cc5</chem> CF_3CO_2H	504.4 (M + H)	3.49

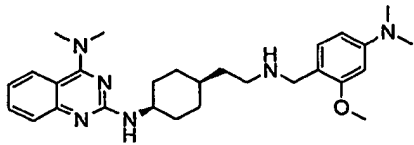
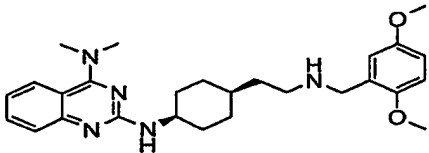
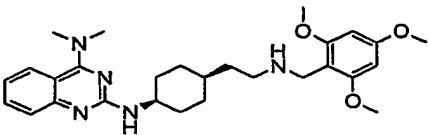
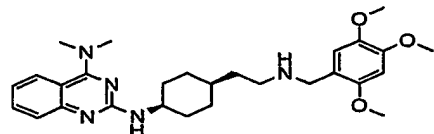
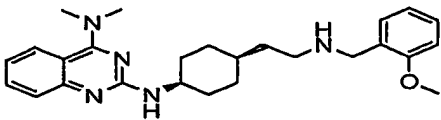
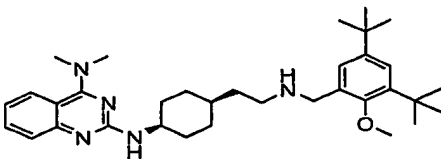
Example No.	Structure	ESI-MS	Retention Time (min)
3161	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4CCCCC4NC(=O)C5=C(C(F)(F)F)OC(=C5)C6=CC=C(C=C6)Cl</chem> <chem>CC(F)(F)C(=O)O</chem>	572.4 (M + H)	3.71
3162	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4=CC=C(C=C4)NC(=O)C5=CC=C(C=C5)C6=CC=CC=C6</chem> <chem>CC(F)(F)C(=O)O</chem>	460.2 (M + H)	3.80
3163	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4=CC=C(C=C4)NC(=O)C5=CC=C(C=C5)C6=CC=CC=C6NC(=O)OC(C)(C)C</chem> <chem>CC(F)(F)C(=O)O</chem>	589.2 (M + H)	4.00
3164	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4=CC=C(C=C4)NC(=O)C5=CC=C(C=C5)C6=CC=C(C=C6)F</chem> <chem>CC(F)(F)C(=O)O</chem>	492.2 (M + H)	3.90
3165	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4=CC=C(C=C4)NC(=O)C5=CC=C(C=C5)C6=CC=C(C=C6)F</chem> <chem>CC(F)(F)C(=O)O</chem>	478.2 (M + H)	3.80
3166	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N(C3)C4=CC=C(C=C4)NC(=O)C5=CC=C(C=C5)C6=CC=C(C=C6)FNC(=O)OC(C)(C)C</chem> <chem>CC(F)(F)C(=O)O</chem>	607.6 (M + H)	4.00

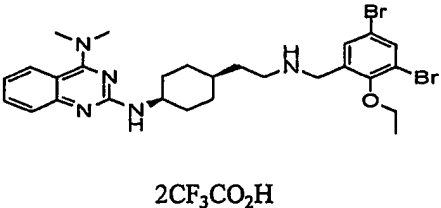
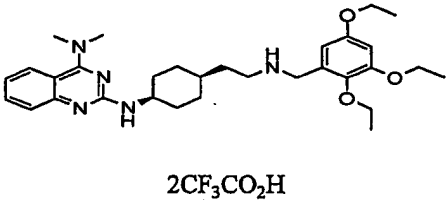
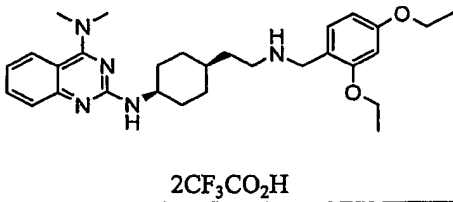
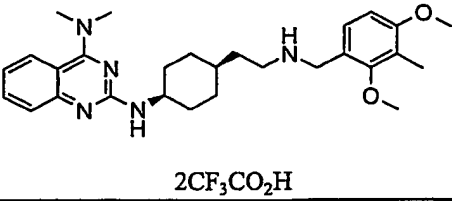
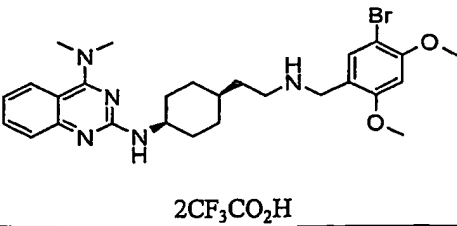
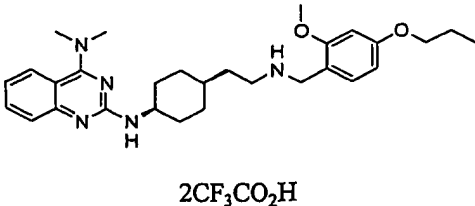
Example No.	Structure	ESI-MS	Retention Time (min)
3167	 <chem>CCN(C)c1nc2c(ncn2C1CNc3ccc(NC(=O)c4ccc(CO)cc4)cc3)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.40
3168	 <chem>Nc1nc2c(ncn2C1CNc3ccc(NC(=O)c4ccc(OS(=O)(=O)C(F)(F)F)cc4)cc3)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.2 (M + H)	3.90
3169	 <chem>CCN(C)c1nc2c(ncn2C1CNc3ccc(NC(=O)c4ccc(C5=CC=CS5)cc4)cc3)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.80
3170	 <chem>Nc1nc2c(ncn2C1CNc3ccc(NC(=O)c4ccc(C5=CC=CS5)cc4)cc3)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.70
3171	 <chem>Nc1nc2c(ncn2C1CNc3ccc(NC(=O)c4c(C)n(C4)SC5=CC=C(Cl)C=C5)cc3)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	515.2 (M + H)	3.90
3172	 <chem>CC(C)(C)OC(=O)NCC1=NC2=CC=CC=C2N=C(N1CNc3ccc(NC(=O)c4c(C)n(C4)SC5=CC=C(Cl)C=C5)cc3)C3=CC=CC=C3N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	4.10

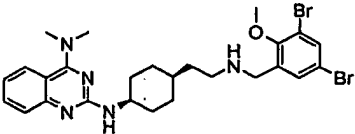
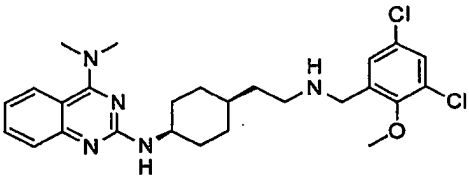
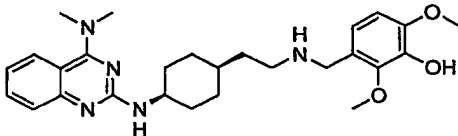
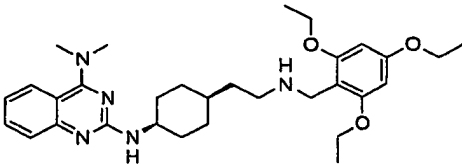
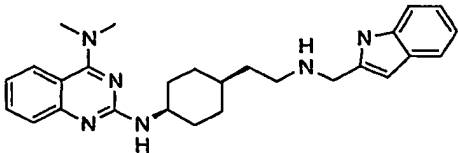
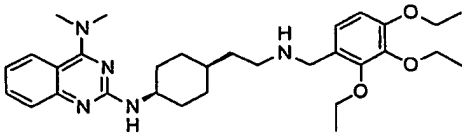
Example No.	Structure	ESI-MS	Retention Time (min)
3173	 <chem>CC1=NC2=CC=CC=C2N1N=C(NCC3=CC=C(NC(=O)CC4=CC=CC=C4C5=CC=CC=C5)C3)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.2 (M + H)	3.90
3174	 <chem>Nc1nc2ccccc2n1NCC3=CC=C(NC(=O)CC4=CC=CC=C4C5=CC=CC=C5)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.80
3175	 <chem>Nc1nc2ccccc2n1NCC3=CC=C(NC(=O)c4cc(Cl)ccc4C5=CC=CC=N5)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	525.4 (M + H)	3.70
3176	 <chem>CC(C)(C)OC(=O)NCC1=NC2=CC=CC=C2N1C(=N)NCC3=CC=C(NC(=O)c4cc(Cl)ccc4C5=CC=CC=N5)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	654.2 (M + H)	3.90
3177	 <chem>CC1=NC2=CC=CC=C2N1N=C(NCC3=CC=C(NC(=O)CC4=CC=C(O)C=C4)C3)C=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	428.2 (M + H)	3.10
3178	 <chem>Nc1nc2ccccc2n1NCC3=CC=C(NC(=O)CC4=CC=C(O)C=C4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	414.4 (M + H)	2.90

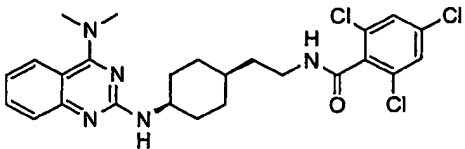
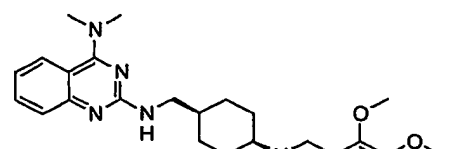
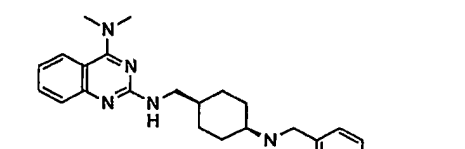
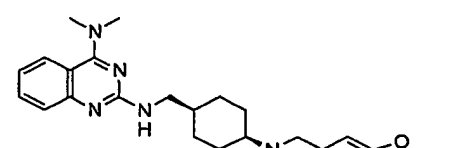
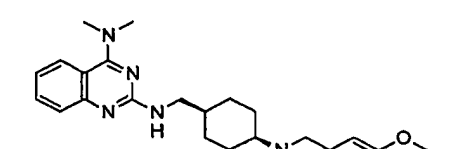
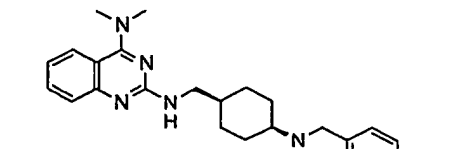
Example No.	Structure	ESI-MS	Retention Time (min)
3179	 $2\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.04
3180	 $2\text{CF}_3\text{CO}_2\text{H}$	578.8 (M + H)	3.50
3181	 $2\text{CF}_3\text{CO}_2\text{H}$	520.6 (M + H)	3.19
3182	 $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.80
3183	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.66
3184	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.66

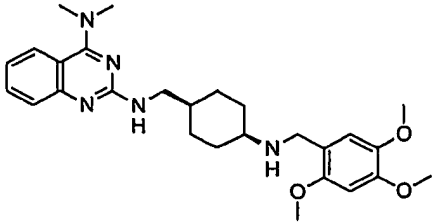
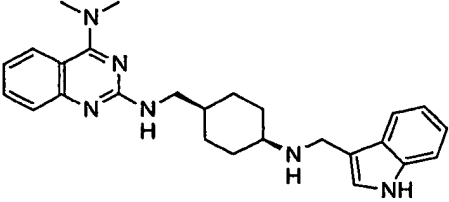
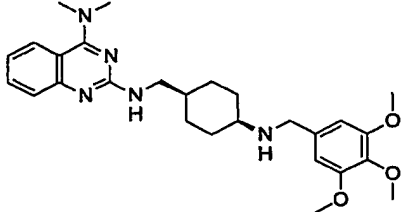
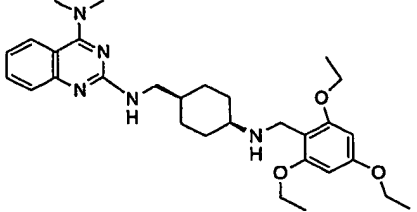
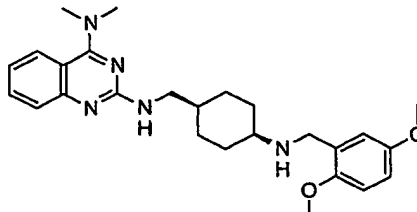
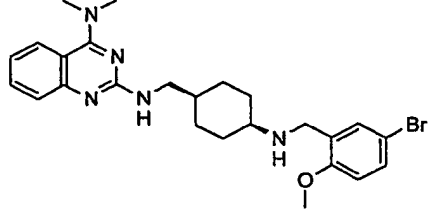
Example No.	Structure	ESI-MS	Retention Time (min)
3185	 <chem>CC1=CN2C(=N1)C(=N2)N[C@@H]3CCCC[C@H]3CCN(Cc4ccc(OC)cc4)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.94
3186	 <chem>COc1cc(OC)ccc1CN(Cc2ccc3c(c2)N[C@@H]4CCCC[C@H]4C(=N3)N5C(=N6C(=N5)C(=N6)N7C8=CC=CC=C8N(C)N7)C8)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.65
3187	 <chem>COc1cc(OC)ccc1CN(Cc2ccc3c(c2)N[C@@H]4CCCC[C@H]4C(=N3)N5C(=N6C(=N5)C(=N6)N7C8=CC=CC=C8N(C)N7)C8)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.68
3188	 <chem>BrC1=CC(OC(F)(F)F)=CC=C1CN(Cc2ccc3c(c2)N[C@@H]4CCCC[C@H]4C(=N3)N5C(=N6C(=N5)C(=N6)N7C8=CC=CC=C8N(C)N7)C8)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	566.4 (M + H)	3.03
3189	 <chem>BrC1=CC(OC)=CC=C1CN(Cc2ccc3c(c2)N[C@@H]4CCCC[C@H]4C(=N3)N5C(=N6C(=N5)C(=N6)N7C8=CC=CC=C8N(C)N7)C8)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	512.6 (M + H)	2.85
3190	 <chem>CC1=CC(C)=CC(C)=C1CN(Cc2ccc3c(c2)N[C@@H]4CCCC[C@H]4C(=N3)N5C(=N6C(=N5)C(=N6)N7C8=CC=CC=C8N(C)N7)C8)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.09

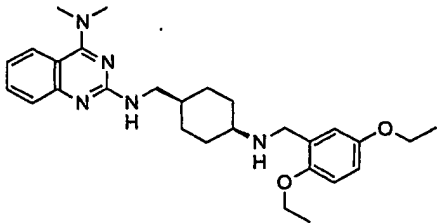
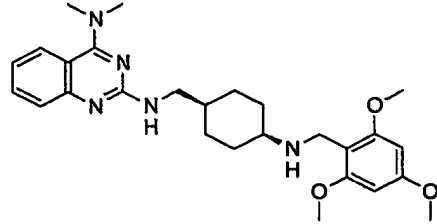
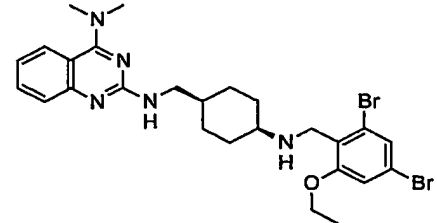
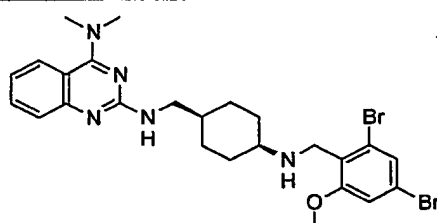
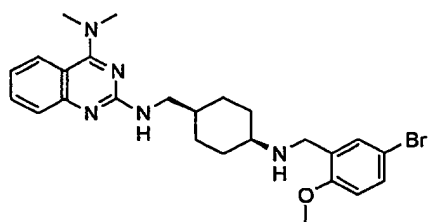
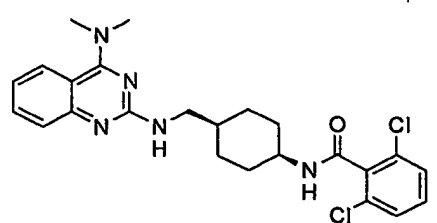
Example No.	Structure	ESI-MS	Retention Time (min)
3191	 $3\text{CF}_3\text{CO}_2\text{H}$	477.4 (M + H)	2.51
3192	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.67
3193	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.78
3194	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.60
3195	 $2\text{CF}_3\text{CO}_2\text{H}$	434.6 (M + H)	2.67
3196	 $2\text{CF}_3\text{CO}_2\text{H}$	546.4 (M + H)	4.30

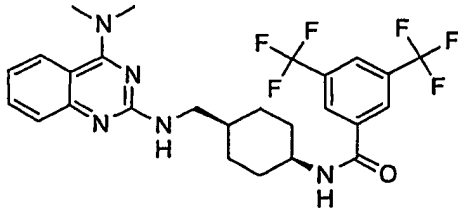
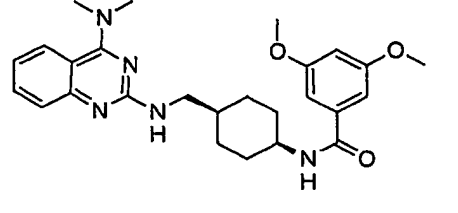
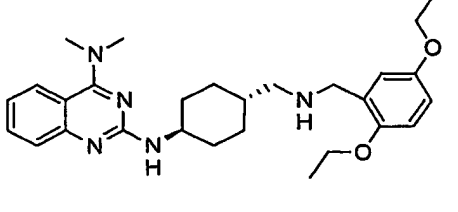
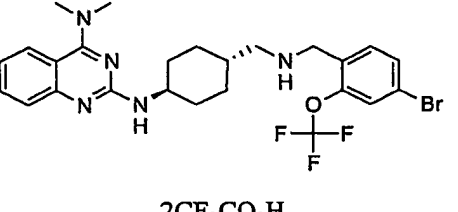
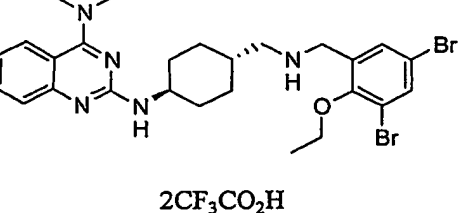
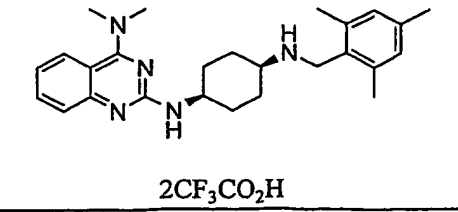
Example No.	Structure	ESI-MS	Retention Time (min)
3197	 $2\text{CF}_3\text{CO}_2\text{H}$	606.6 (M + H)	3.95
3198	 $2\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	3.83
3199	 $2\text{CF}_3\text{CO}_2\text{H}$	492.4 (M + H)	2.97
3200	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.79
3201	 $2\text{CF}_3\text{CO}_2\text{H}$	542.0 (M + H)	2.85
3202	 $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.81

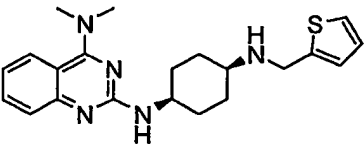
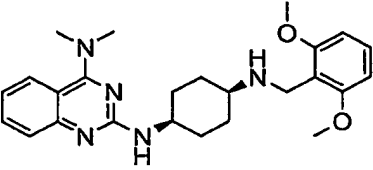
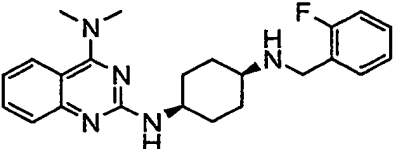
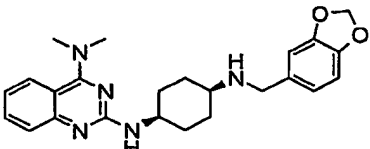
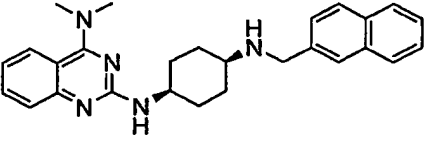
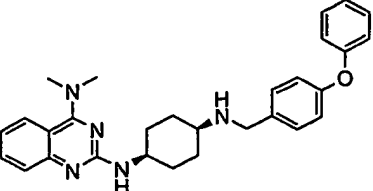
Example No.	Structure	ESI-MS	Retention Time (min)
3203	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=CC(=C(C=C4)Br)Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	590.4 (M + H)	3.02
3204	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=CC(=C(C=C4)Cl)ClOC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	2.91
3205	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=CC(=C(C=C4)OC)OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.51
3206	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=CC(=C(C=C4)OCC)OCC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.21
3207	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=Cc5ccccc5n4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	443.6 (M + H)	2.66
3208	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3CCNCC4=CC(=C(C=C4)OCC)OCC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.08

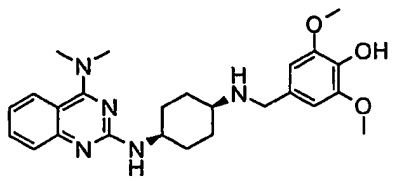
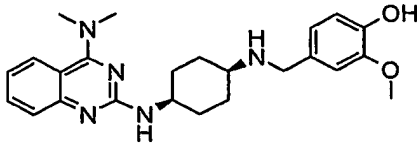
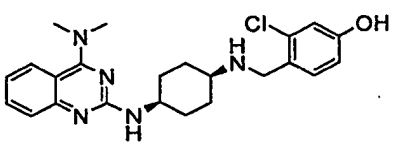
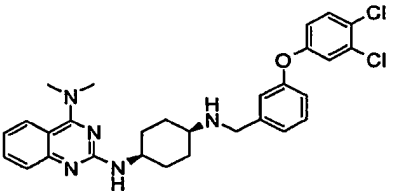
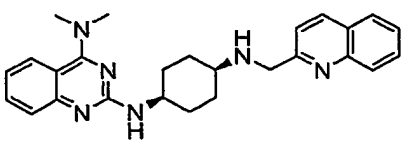
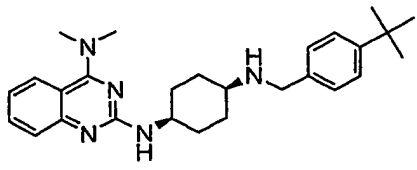
Example No.	Structure	ESI-MS	Retention Time (min)
3209	 <chem>CCN(C)c1nc2c(ncn2C3CCCCC3CNC(=O)c4cc(Cl)cc(Cl)c4Cl)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	520.0 (M + H)	3.51
3210	 <chem>COc1cc(OC)c(OC)c(CNC2CCCCC2CNC3=NC4=CC=CC=C4N(C)C3)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.58
3211	 <chem>Brc1cc(C(F)(F)F)ccc(CNC2CCCCC2CNC3=NC4=CC=CC=C4N(C)C3)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.11
3212	 <chem>COC1=CC=C2C(=C1)OCOC2CNC3CCCCC3CNC4=NC5=CC=CC=C5N(C)C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.22
3213	 <chem>COc1cc(CNC2CCCCC2CNC3=NC4=CC=CC=C4N(C)C3)cc(OC)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.70
3214	 <chem>COc1cc(CNC2CCCCC2CNC3=NC4=CC=CC=C4N(C)C3)cc(OC)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.58

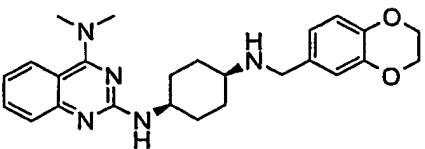
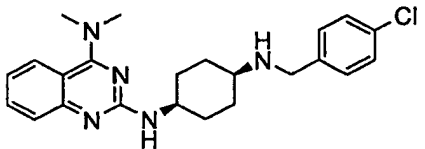
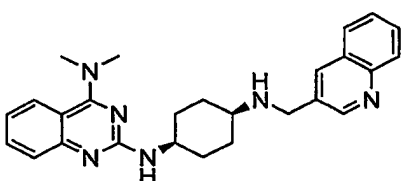
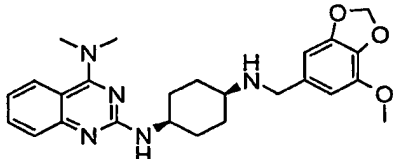
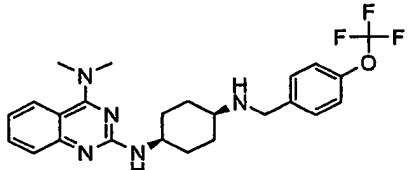
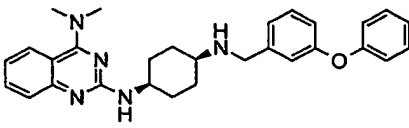
Example No.	Structure	ESI-MS	Retention Time (min)
3215	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.73
3216	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $3\text{CF}_3\text{CO}_2\text{H}$	429.4 (M + H)	3.29
3217	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.78
3218	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	3.77
3219	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.2 (M + H)	2.57
3220	 <chem>COc1ccc(cc1)CN(CCN(C)Nc2ccccc2n3nc(NCC4CCCCC4NCC5=CC(OC)=CC(OC)=C5)nc3)CC6=CC(OC)=CC(OC)=C6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	498.0 (M + H)	2.97

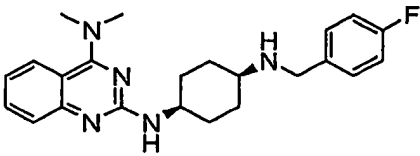
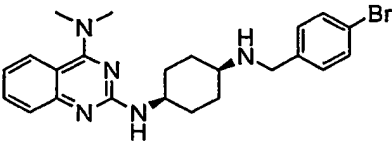
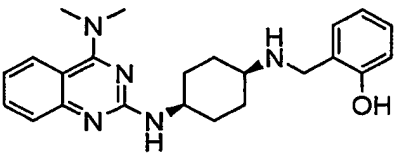
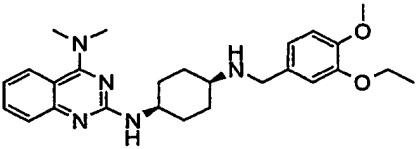
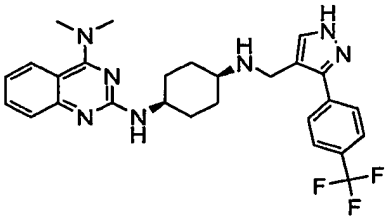
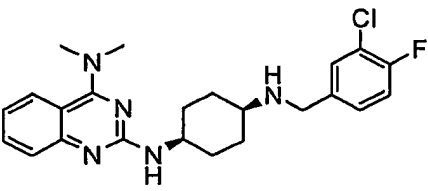
Example No.	Structure	ESI-MS	Retention Time (min)
3221	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.17
3222	 $2\text{CF}_3\text{CO}_2\text{H}$	480.0 (M + H)	3.08
3223	 $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	4.20
3224	 $2\text{CF}_3\text{CO}_2\text{H}$	576.4 (M + H)	3.95
3225	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.86
3226	 $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.07

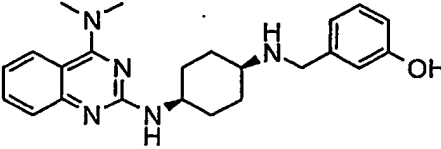
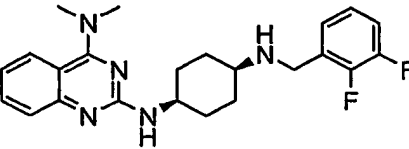
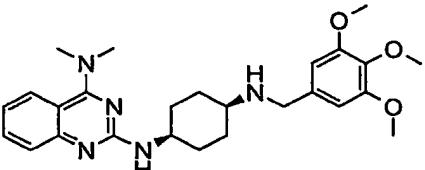
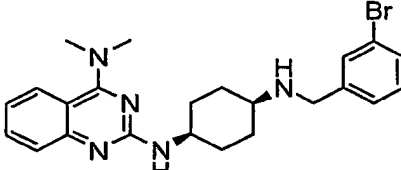
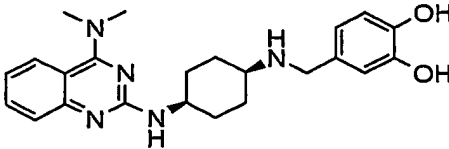
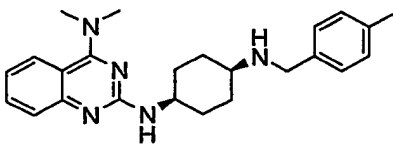
Example No.	Structure	ESI-MS	Retention Time (min)
3227	 $\text{CF}_3\text{CO}_2\text{H}$	540.6 (M + H)	3.75
3228	 $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.07
3229	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.40
3230	 $2\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	3.50
3231	 $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	3.60
3232	 $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.25

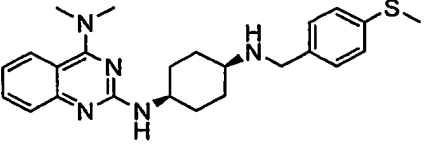
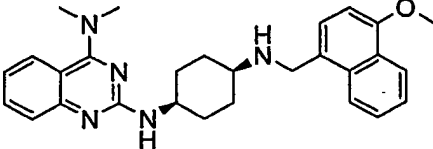
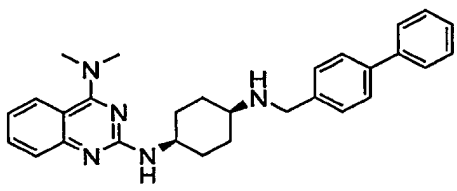
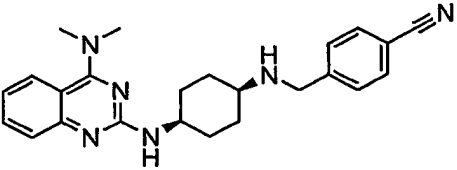
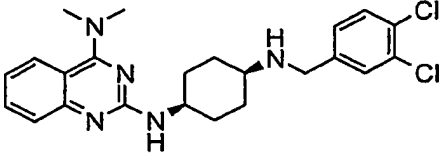
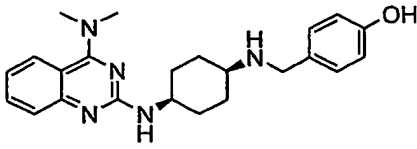
Example No.	Structure	ESI-MS	Retention Time (min)
3233	 $2\text{CF}_3\text{CO}_2\text{H}$	382.2 (M + H)	2.67
3234	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.05
3235	 $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.75
3236	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.82
3237	 $2\text{CF}_3\text{CO}_2\text{H}$	426.4 (M + H)	3.17
3238	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.44

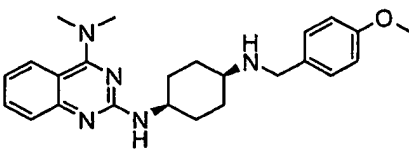
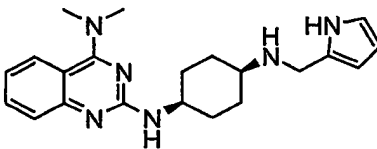
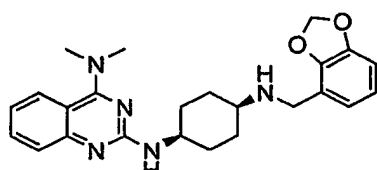
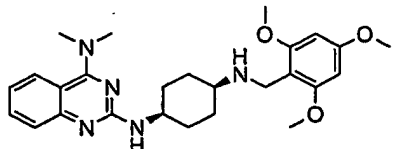
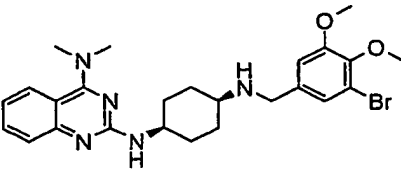
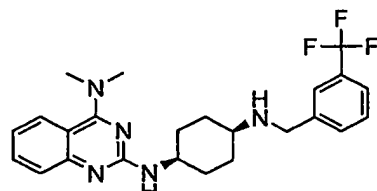
Example No.	Structure	ESI-MS	Retention Time (min)
3239	 2CF ₃ CO ₂ H	452.2 (M + H)	2.69
3240	 2CF ₃ CO ₂ H	436.4 (M + H)	2.80
3241	 2CF ₃ CO ₂ H	426.2 (M + H)	2.79
3242	 2CF ₃ CO ₂ H	536.4 (M + H)	3.75
3243	 3CF ₃ CO ₂ H	427.2 (M + H)	2.95
3244	 2CF ₃ CO ₂ H	432.4 (M + H)	3.41

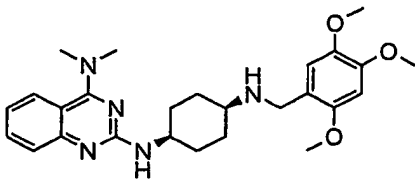
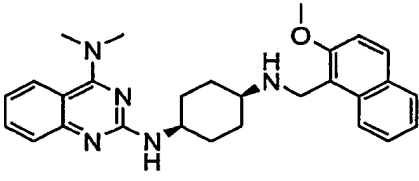
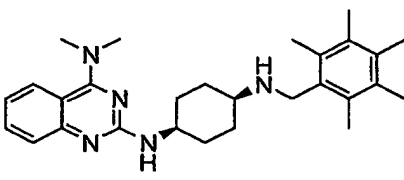
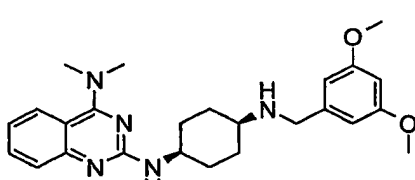
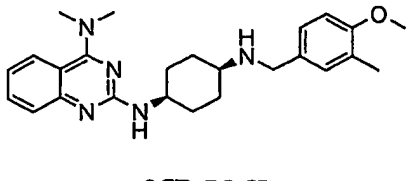
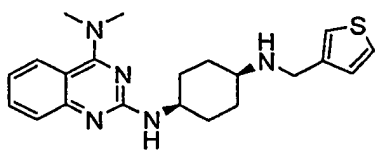
Example No.	Structure	ESI-MS	Retention Time (min)
3245	 $2\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	2.84
3246	 $2\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.02
3247	 $3\text{CF}_3\text{CO}_2\text{H}$	427.4 (M + H)	2.61
3248	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.91
3249	 $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.19
3250	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.79

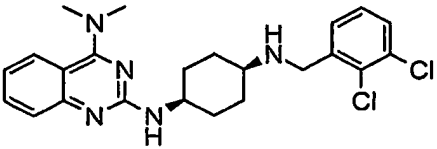
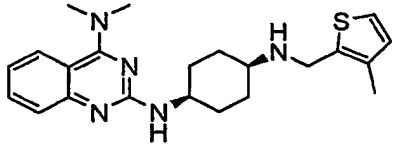
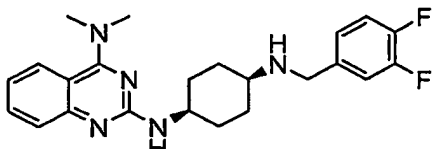
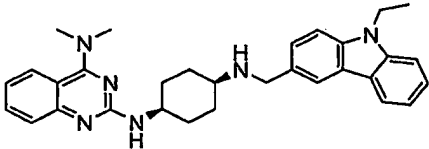
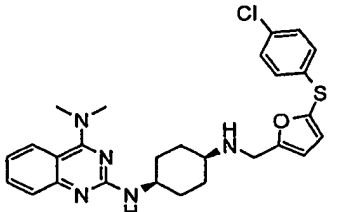
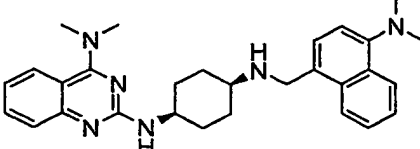
Example No.	Structure	ESI-MS	Retention Time (min)
3251	 $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.83
3252	 $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.08
3253	 $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.73
3254	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.92
3255	 $3\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
3256	 $2\text{CF}_3\text{CO}_2\text{H}$	428.2 (M + H)	3.08

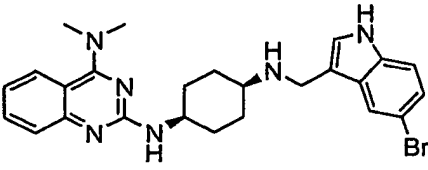
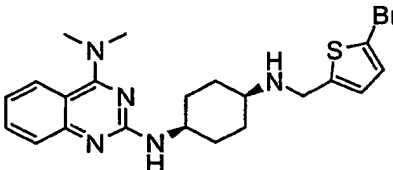
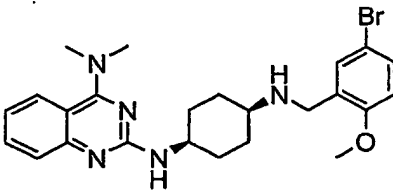
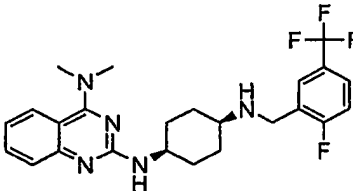
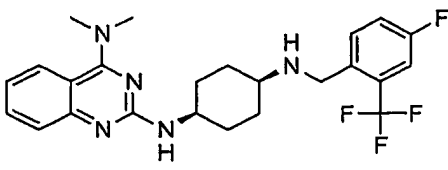
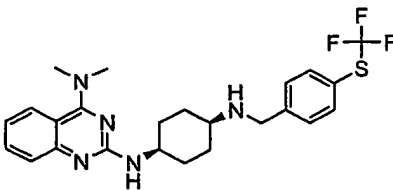
Example No.	Structure	ESI-MS	Retention Time (min)
3257	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(O)C=C4.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	392.4 (M + H)	2.63
3258	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)F)F.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	412.2 (M + H)	2.83
3259	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(OC)=C(OC)C(OC)=C4.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	466.4 (M + H)	2.89
3260	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(Br)C=C4.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	454.0 (M + H)	3.05
3261	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)O)O.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	408.2 (M + H)	2.53
3262	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(C)C=C4.CC(F)(F)C(=O)O.CC(F)(F)C(=O)O</chem>	390.4 (M + H)	2.92

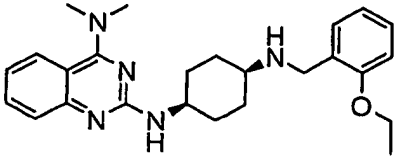
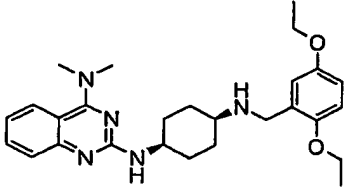
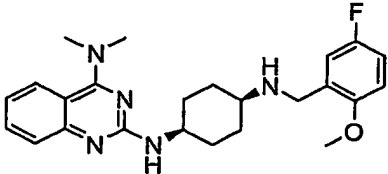
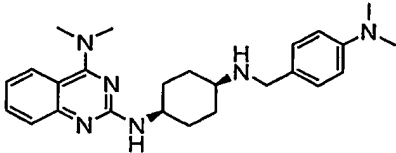
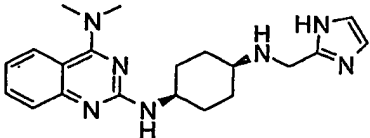
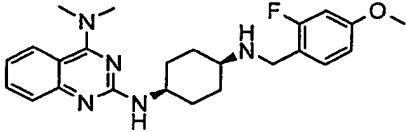
Example No.	Structure	ESI-MS	Retention Time (min)
3263	 $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.05
3264	 $2\text{CF}_3\text{CO}_2\text{H}$	456.4 (M + H)	3.25
3265	 $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	3.37
3266	 $2\text{CF}_3\text{CO}_2\text{H}$	401.2 (M + H)	2.76
3267	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.17
3268	 $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.61

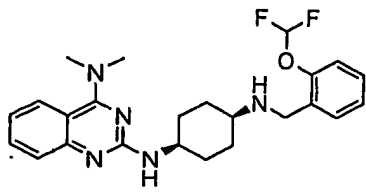
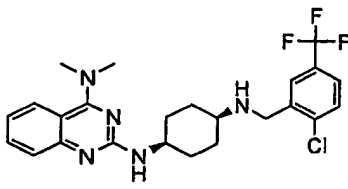
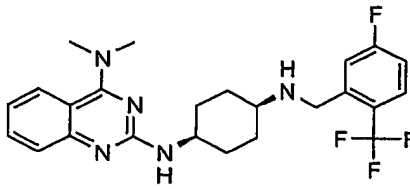
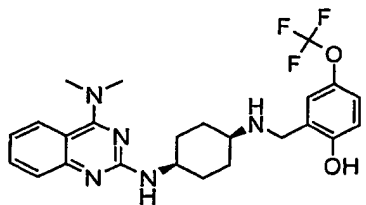
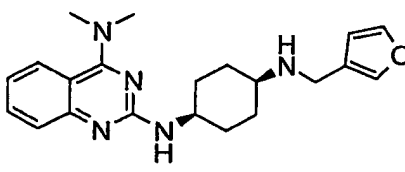
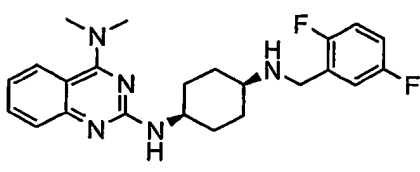
Example No.	Structure	ESI-MS	Retention Time (min)
3269	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.86
3270	 $3\text{CF}_3\text{CO}_2\text{H}$	365.4 (M + H)	2.61
3271	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.83
3272	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.10
3273	 $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.13
3274	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.17

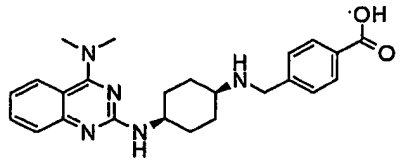
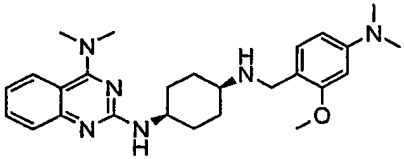
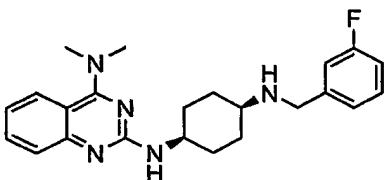
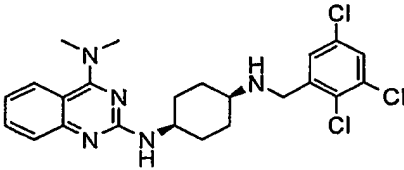
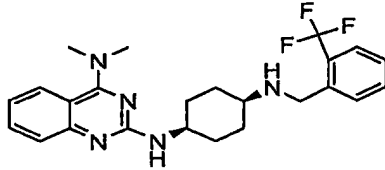
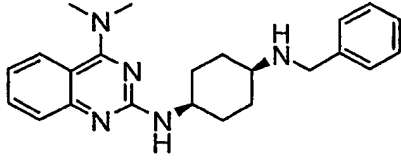
Example No.	Structure	ESI-MS	Retention Time (min)
3275	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>COc1ccc(cc1)CN[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	466.4 (M + H)	2.86
3276	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>COc1ccc(cc1)CN[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	456.2 (M + H)	3.22
3277	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>CC1=CC(C)=CC(C)=C1CN[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	446.6 (M + H)	3.45
3278	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>COc1cc(OC)ccc1CN[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	436.4 (M + H)	2.95
3279	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>COc1ccc(cc1)CN[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	420.2 (M + H)	3.03
3280	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)N(C)C</chem> <chem>C1=CC=C(C=C1)S[C@H]2CCCC[C@H]2N[C@@H]3C4=CC(=CC=C4)N(C)C(=N3)N(C)C</chem> <chem>2CF3CO2H</chem>	382.4 (M + H)	2.72

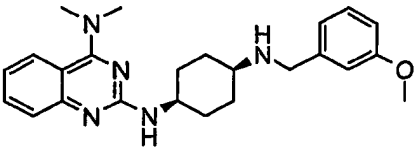
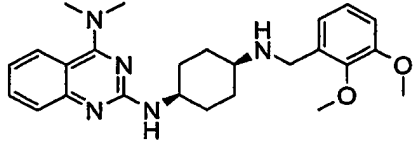
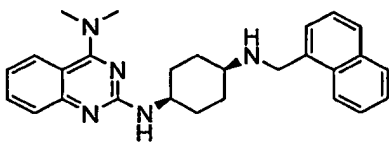
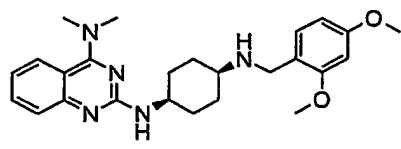
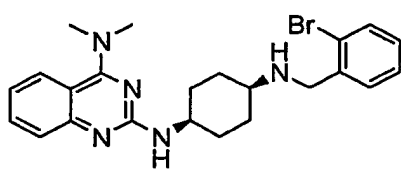
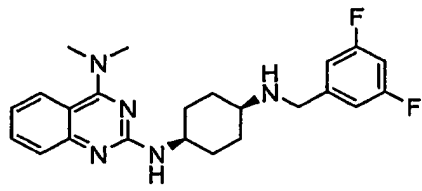
Example No.	Structure	ESI-MS	Retention Time (min)
3281	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.07
3282	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.79
3283	 $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.95
3284	 $32\text{CF}_3\text{CO}_2\text{H}$	493.4 (M + H)	3.57
3285	 $2\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.52
3286	 $2\text{CF}_3\text{CO}_2\text{H}$	469.6 (M + H)	2.76

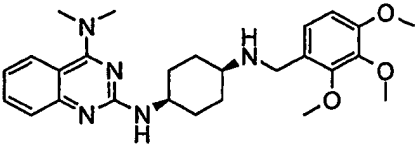
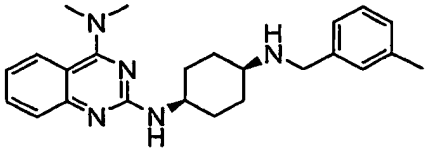
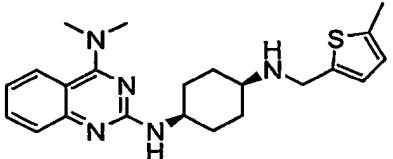
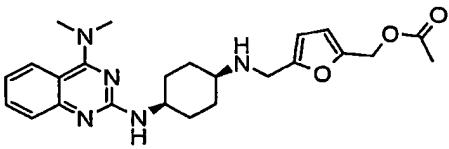
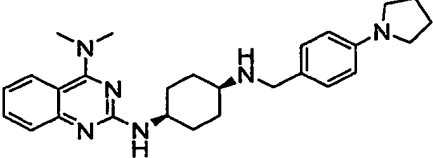
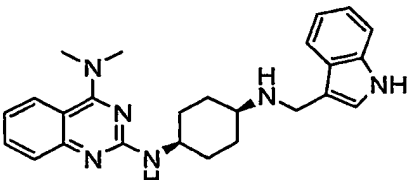
Example No.	Structure	ESI-MS	Retention Time (min)
3287	 3CF ₃ CO ₂ H	493.2 (M + H)	3.17
3288	 2CF ₃ CO ₂ H	460.2 (M + H)	2.95
3289	 2CF ₃ CO ₂ H	484.2 (M + H)	3.14
3290	 2CF ₃ CO ₂ H	462.2 (M + H)	3.11
3291	 2CF ₃ CO ₂ H	462.2 (M + H)	3.11
3292	 2CF ₃ CO ₂ H	476.4 (M + H)	3.39

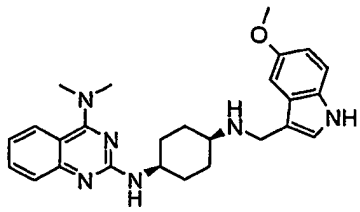
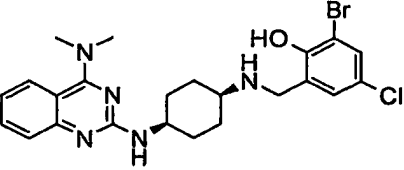
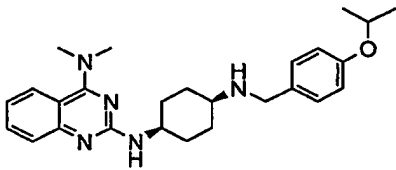
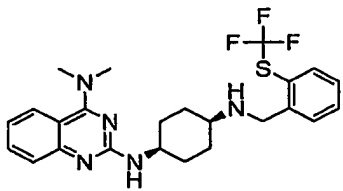
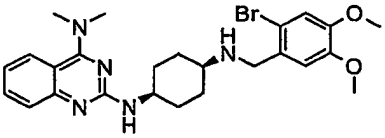
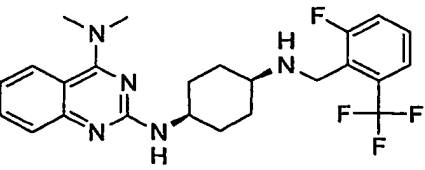
Example No.	Structure	ESI-MS	Retention Time (min)
3293	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	3.05
3294	 $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.21
3295	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.94
3296	 $3\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	2.51
3297	 $3\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.26
3298	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.93

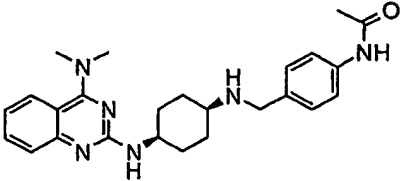
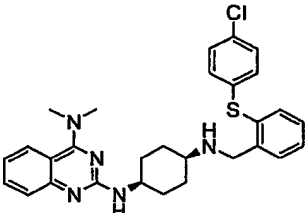
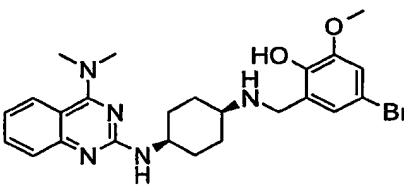
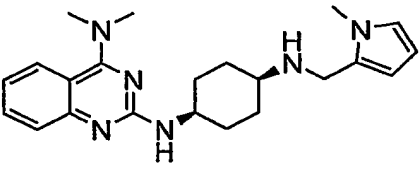
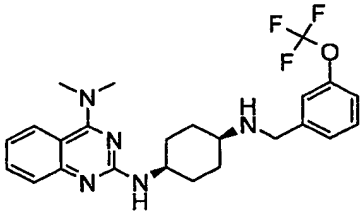
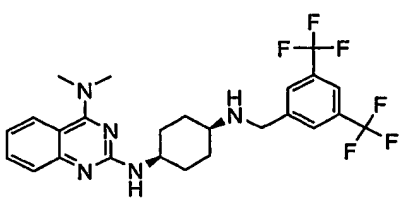
Example No.	Structure	ESI-MS	Retention Time (min)
3299	 $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	2.97
3300	 $2\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.19
3301	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.05
3302	 $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.20
3303	 $2\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.64
3304	 $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.85

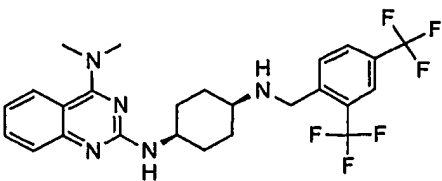
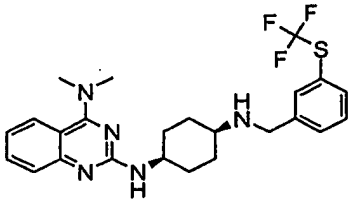
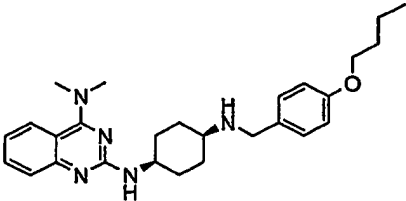
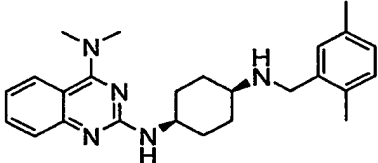
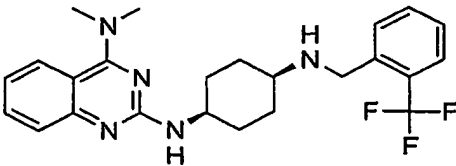
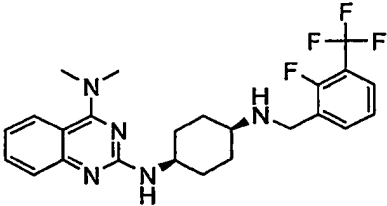
Example No.	Structure	ESI-MS	Retention Time (min)
3305	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4ccc(C(=O)O)cc4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.67
3306	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4cc(OC)c(N(C)C)cc4)c5ccccc15</chem> $3\text{CF}_3\text{CO}_2\text{H}$	449.4 (M + H)	2.74
3307	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4ccc(F)cc4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.86
3308	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4cc(Cl)c(Cl)c(Cl)c4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.38
3309	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4cc(F)(F)c5ccccc45)c6ccccc16</chem> $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.09
3310	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4ccccc4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	376.4 (M + H)	2.82

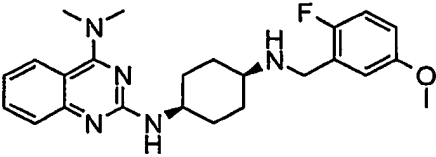
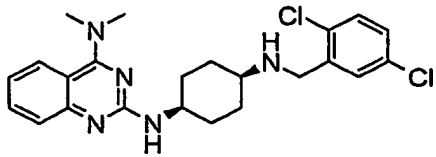
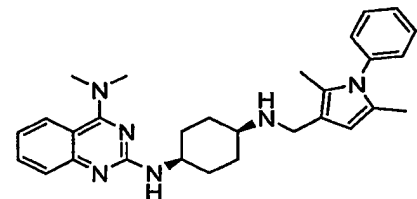
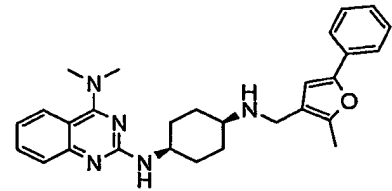
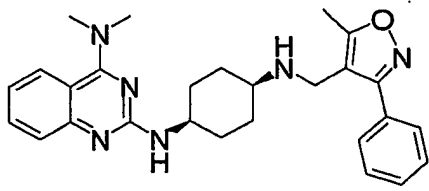
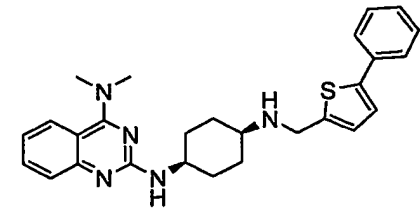
Example No.	Structure	ESI-MS	Retention Time (min)
3311	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.87
3312	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.91
3313	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.13
3314	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.99
3315	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	2.97
3316	 <chem>CN(C)c1nc2c(ncn2CNC3C=CC=CC=C3)nc4ccccc14</chem> $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.92

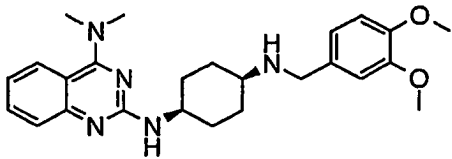
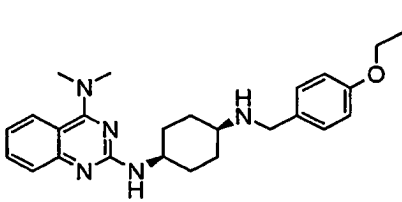
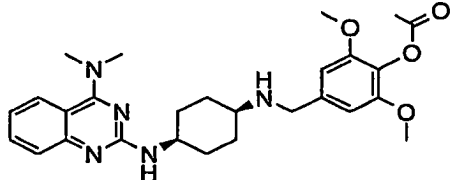
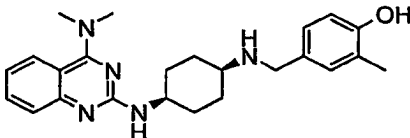
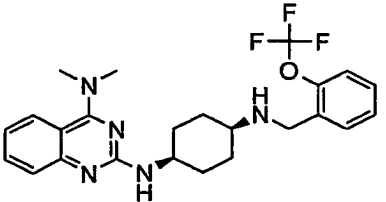
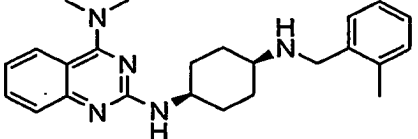
Example No.	Structure	ESI-MS	Retention Time (min)
3317	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.95
3318	 $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.95
3319	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.89
3320	 $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.76
3321	 $3\text{CF}_3\text{CO}_2\text{H}$	445.4 (M + H)	3.16
3322	 $3\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.96

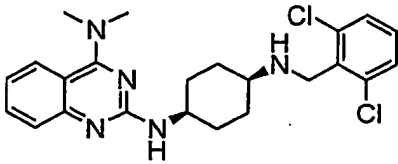
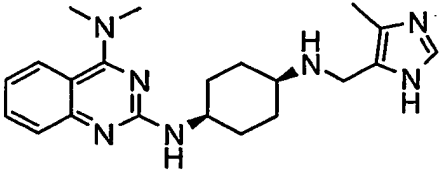
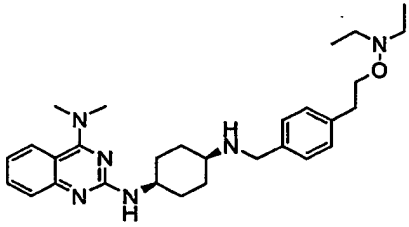
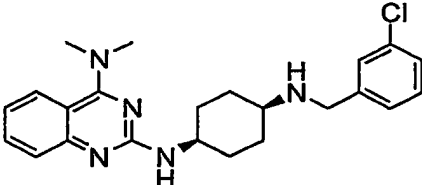
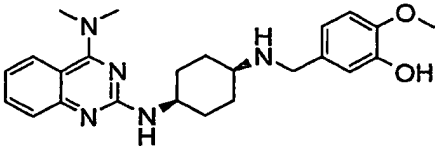
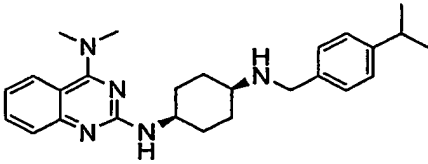
Example No.	Structure	ESI-MS	Retention Time (min)
3323	 <chem>CCN(C)c1nc2c(ncn2C1Cc3ccccc3)nc4cnc5c4nc6c5cnc6N(C)C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	445.4 (M + H)	2.96
3324	 <chem>CCN(C)c1nc2c(ncn2C1Cc3ccccc3)nc4cnc5c4nc6c5cnc6N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.11
3325	 <chem>CC(C)Oc1ccc(cc1)Cc2nc3c(ncn3C2Cc4ccccc4)nc5cnc6c5cnc6N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.17
3326	 <chem>CCN(C)c1nc2c(ncn2C1Cc3ccccc3)nc4cnc5c4nc6c5cnc6N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.27
3327	 <chem>COc1cc(Br)cc(OC)c1Cc2nc3c(ncn3C2Cc4ccccc4)nc5cnc6c5cnc6N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.07
3328	 <chem>Fc1cc(C(F)(F)F)ccc1Cc2nc3c(ncn3C2Cc4ccccc4)nc5cnc6c5cnc6N(C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	2.99

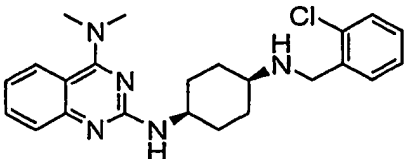
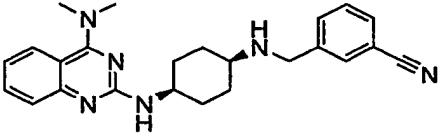
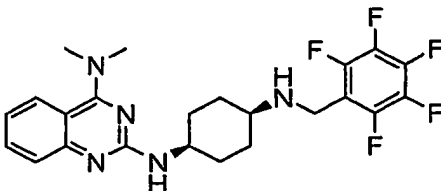
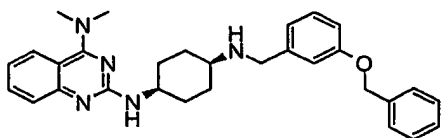
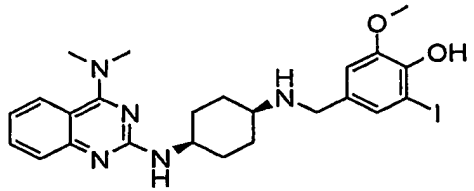
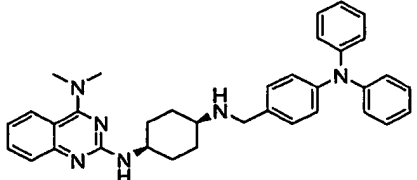
Example No.	Structure	ESI-MS	Retention Time (min)
3329	 $2\text{CF}_3\text{CO}_2\text{H}$	433.2 (M + H)	2.63
3330	 $2\text{CF}_3\text{CO}_2\text{H}$	518.4 (M + H)	3.63
3331	 $2\text{CF}_3\text{CO}_2\text{H}$	500.4 (M + H)	3.09
3332	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.77
3333	 $2\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	3.31
3334	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.51

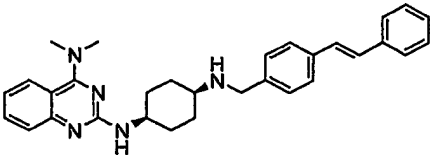
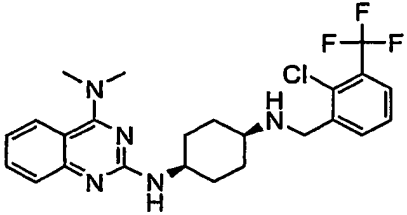
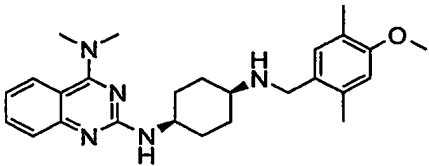
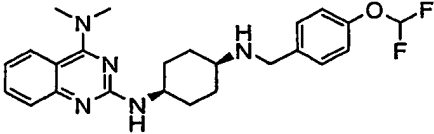
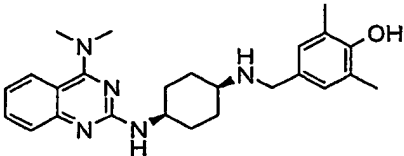
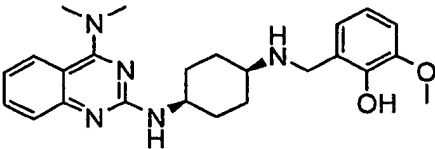
Example No.	Structure	ESI-MS	Retention Time (min)
3335	 $2\text{CF}_3\text{CO}_2\text{H}$	512.6 (M + H)	3.51
3336	 $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.39
3337	 $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.42
3338	 $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.17
3339	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.13
3340	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.21

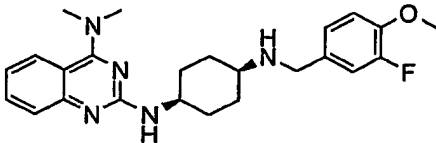
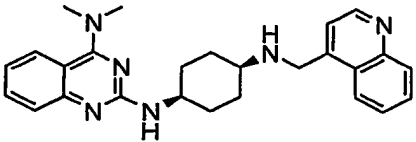
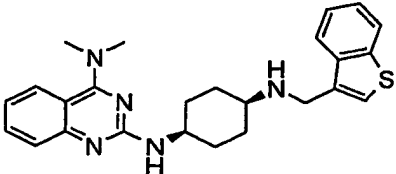
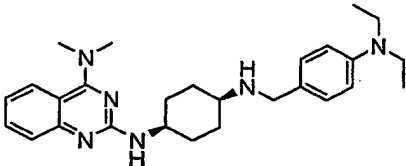
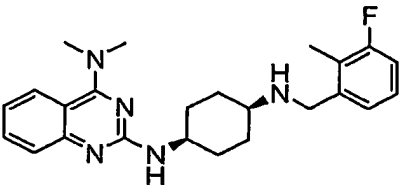
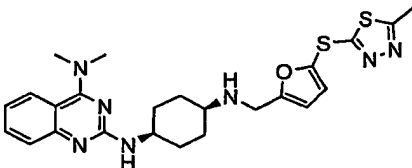
Example No.	Structure	ESI-MS	Retention Time (min)
3341	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.97
3342	 $2\text{CF}_3\text{CO}_2\text{H}$	444.6 (M + H)	3.16
3343	 $3\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	3.47
3344	 $2\text{CF}_3\text{CO}_2\text{H}$	456.4 (M + H)	3.47
3345	 $2\text{CF}_3\text{CO}_2\text{H}$	457.4 (M + H)	3.09
3346	 $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.37

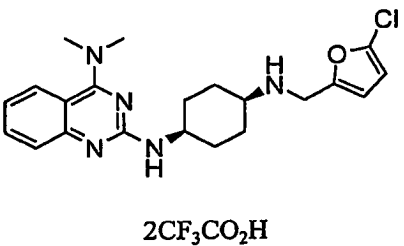
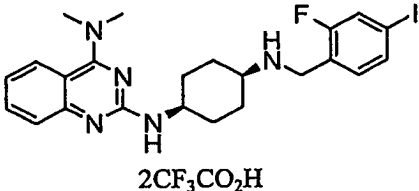
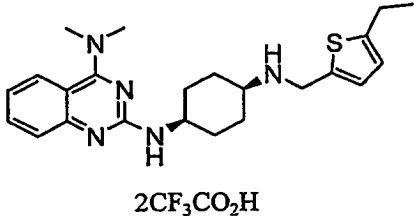
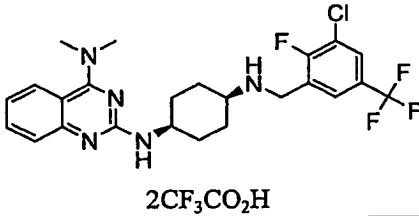
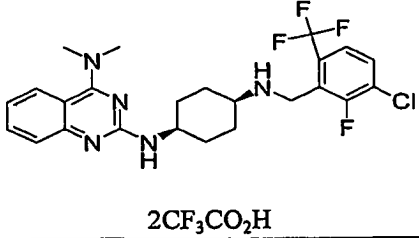
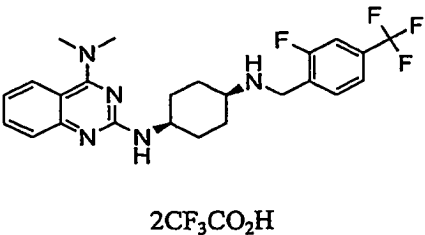
Example No.	Structure	ESI-MS	Retention Time (min)
3347	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NCc4ccc(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.83
3348	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NCc4ccc(OCC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30
3349	 <chem>CC(=O)Oc1c(OC)c(OC)cc(CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.98
3350	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NCc4ccc(O)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
3351	 <chem>COc1ccc(CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n(C)c3)cc1C(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.20
3352	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NCc4ccccc4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.97

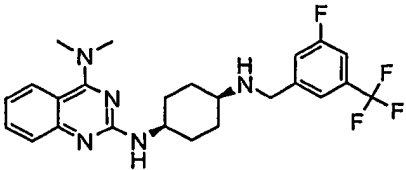
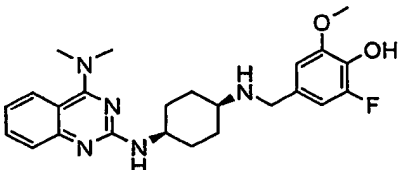
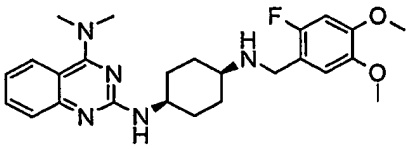
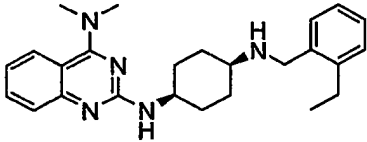
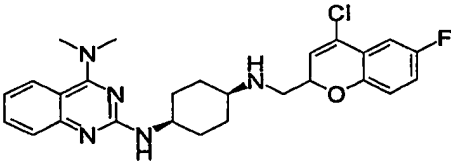
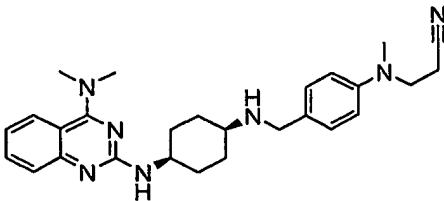
Example No.	Structure	ESI-MS	Retention Time (min)
3353	 $2\text{CF}_3\text{CO}_2\text{H}$	444.2 (M + H)	3.01
3354	 $3\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.27
3355	 $2\text{CF}_3\text{CO}_2\text{H}$	491.4 (M + H)	2.55
3356	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.05
3357	 $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	2.69
3358	 $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.36

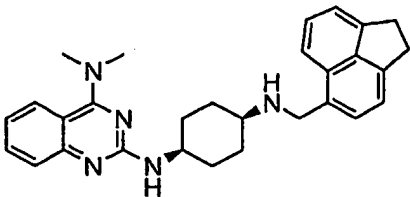
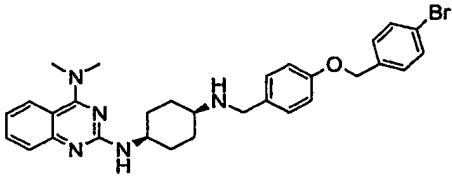
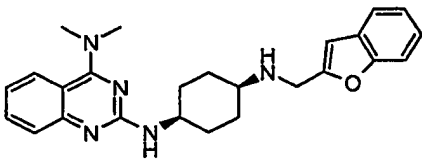
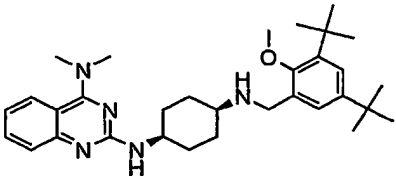
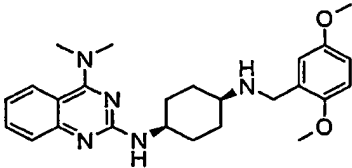
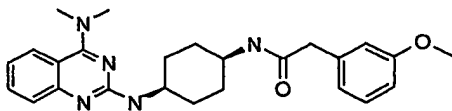
Example No.	Structure	ESI-MS	Retention Time (min)
3359	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.97
3360	 $2\text{CF}_3\text{CO}_2\text{H}$	401.2 (M + H)	2.81
3361	 $2\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.01
3362	 $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
3363	 $2\text{CF}_3\text{CO}_2\text{H}$	548.4 (M + H)	3.03
3364	 $3\text{CF}_3\text{CO}_2\text{H}$	543.6 (M + H)	3.95

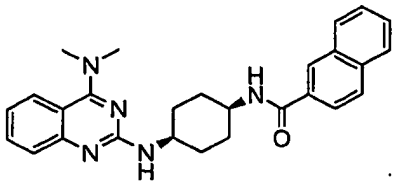
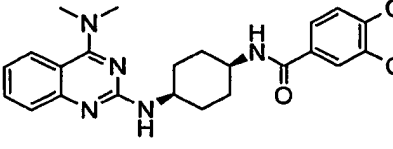
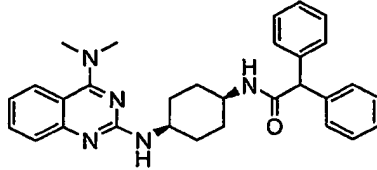
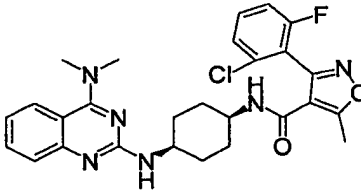
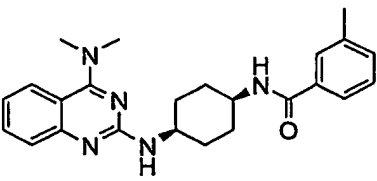
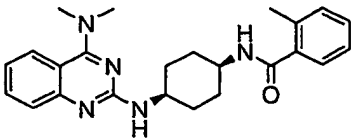
Example No.	Structure	ESI-MS	Retention Time (min)
3365	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.64
3366	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.29
3367	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.20
3368	 $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	3.09
3369	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.87
3370	 $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	2.79

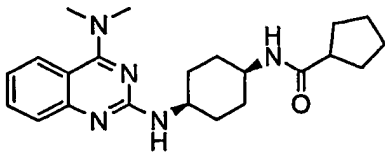
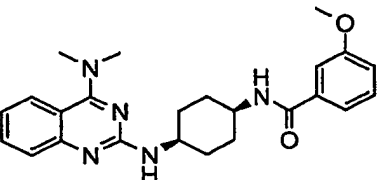
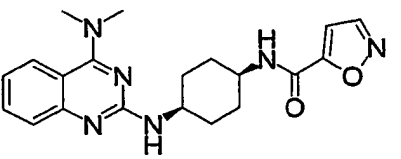
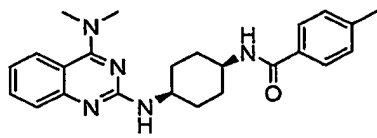
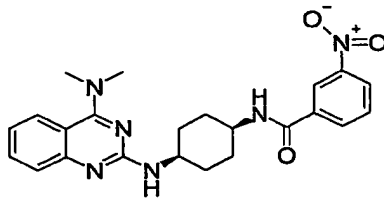
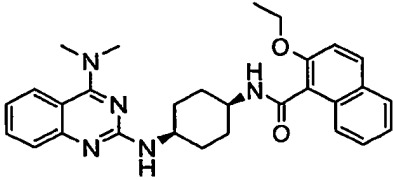
Example No.	Structure	ESI-MS	Retention Time (min)
3371	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.96
3372	 $3\text{CF}_3\text{CO}_2\text{H}$	427.2 (M + H)	2.53
3373	 $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.12
3374	 $3\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	2.45
3375	 $2\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	3.02
3376	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	2.81

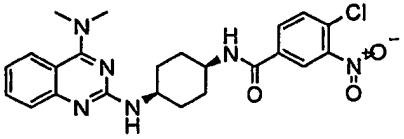
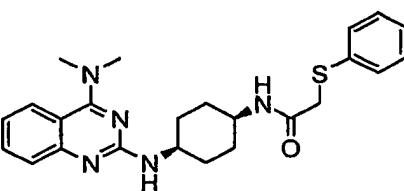
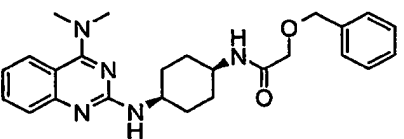
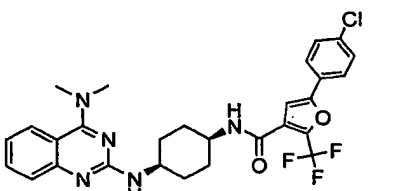
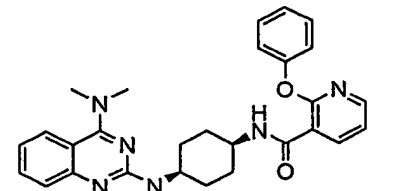
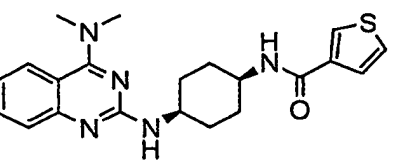
Example No.	Structure	ESI-MS	Retention Time (min)
3377	 $2\text{CF}_3\text{CO}_2\text{H}$	400.2 (M + H)	2.81
3378	 $2\text{CF}_3\text{CO}_2\text{H}$	520.2 (M + H)	3.14
3379	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.12
3380	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.40
3381	 $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.17
3382	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.19

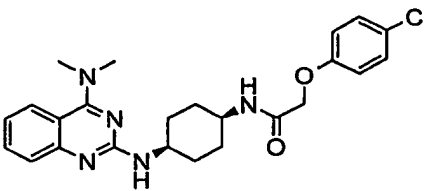
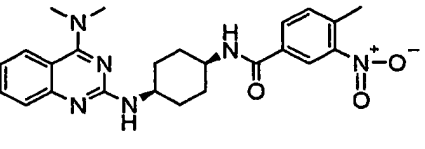
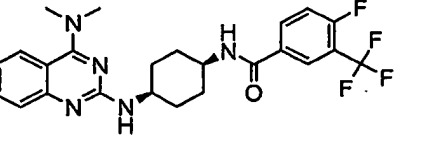
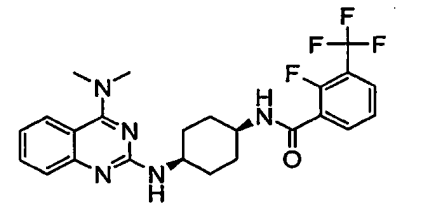
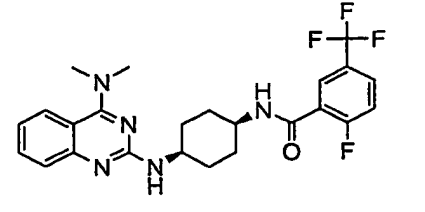
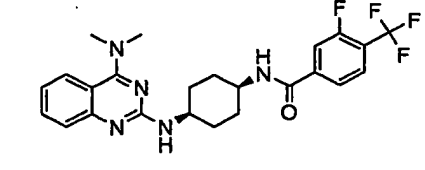
Example No.	Structure	ESI-MS	Retention Time:(min)
3383	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.28
3384	 $2\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	2.74
3385	 $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.89
3386	 $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.09
3387	 $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.29
3388	 $3\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	2.99

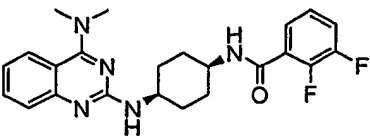
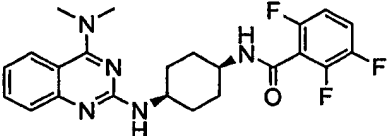
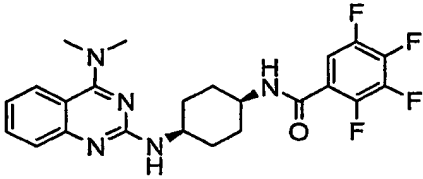
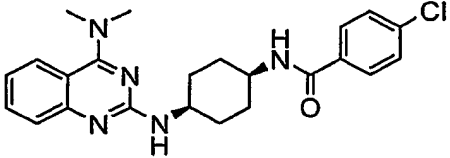
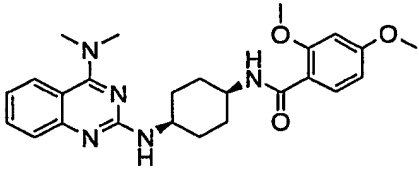
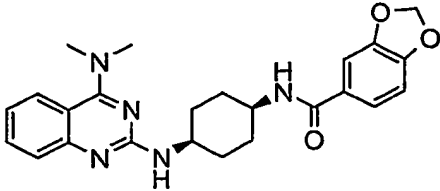
Example No.	Structure	ESI-MS	Retention Time (min)
3389	 $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	3.40
3390	 $2\text{CF}_3\text{CO}_2\text{H}$	560.2 (M + H)	3.73
3391	 $2\text{CF}_3\text{CO}_2\text{H}$	416.4 (M + H)	2.99
3392	 $2\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.08
3393	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.95
3394	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30

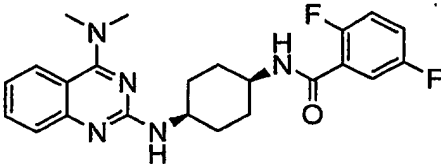
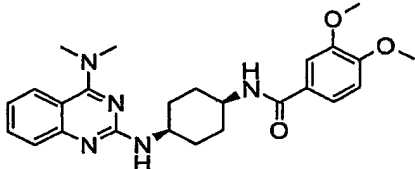
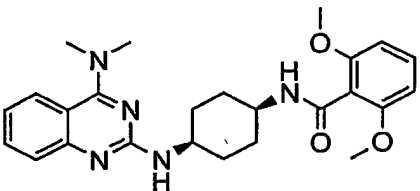
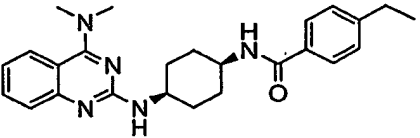
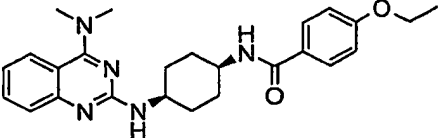
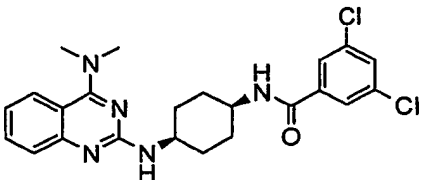
Example No.	Structure	ESI-MS	Retention Time (min)
3395	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)c3ccccc3)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.26
3396	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)c3cc(Cl)cc(Cl)c3)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.39
3397	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)C(c3ccccc3)c4ccccc4)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.37
3398	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)N3C(=O)C4=CC=CC=C4C(F)=CC3O)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	523.6 (M + H)	4.15
3399	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)c3ccc(C)cc3)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.46
3400	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC(=O)c3ccccc3)C4CCCCC4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.75

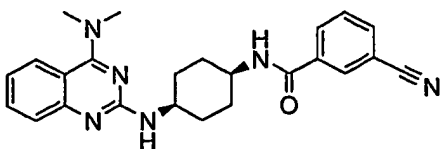
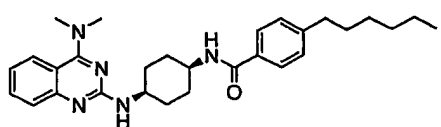
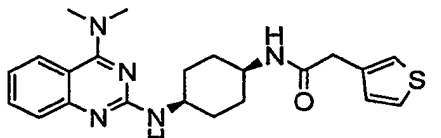
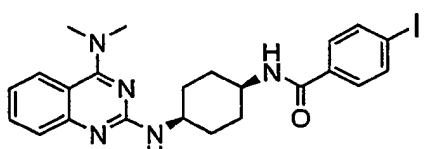
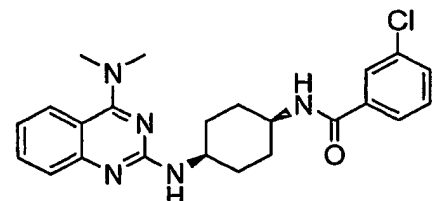
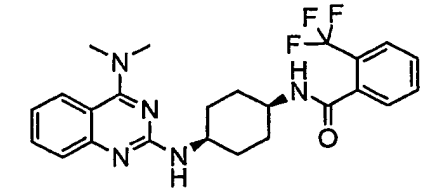
Example No.	Structure	ESI-MS	Retention Time (min)
3401	 <chem>CC1(C)N2C=NC3=C(NC(=O)N[C@H]1CCCC[C@H]3C(=O)N4CCCC4)C=CC=C2</chem> <chem>CC(F)(F)C(=O)O</chem>	382.4 (M + H)	3.65
3402	 <chem>COc1ccc(cc1)C(=O)N[C@H]1CCCC[C@H]2C(=O)N[C@@H]1C3=NC4=C(N(C)C)C=CC=C4N3</chem> <chem>CC(F)(F)C(=O)O</chem>	420.4 (M + H)	3.81
3403	 <chem>C1=CC=C2C(=C1)N(C)N2C3=NC4=CC=CC=C4N3C(=O)N[C@H]1CCCC[C@H]2C(=O)N5C=CC=C5O</chem> <chem>CC(F)(F)C(=O)O</chem>	381.2 (M + H)	3.33
3404	 <chem>CC1=CC=C(C=C1)C(=O)N[C@H]1CCCC[C@H]2C(=O)N[C@@H]1C3=NC4=C(N(C)C)C=CC=C4N3</chem> <chem>CC(F)(F)C(=O)O</chem>	404.4 (M + H)	3.93
3405	 <chem>[O-][N+](=O)c1ccc(cc1)C(=O)N[C@H]1CCCC[C@H]2C(=O)N[C@@H]1C3=NC4=C(N(C)C)C=CC=C4N3</chem> <chem>CC(F)(F)C(=O)O</chem>	435.2 (M + H)	3.40
3406	 <chem>CCOC1=CC2=C(C=C1)C=CC=CC2C(=O)N[C@H]1CCCC[C@H]2C(=O)N[C@@H]1C3=NC4=C(N(C)C)C=CC=C4N3</chem> <chem>CC(F)(F)C(=O)O</chem>	484.4 (M + H)	4.15

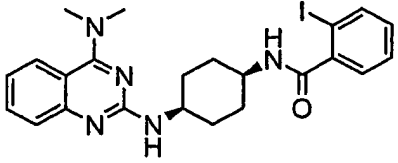
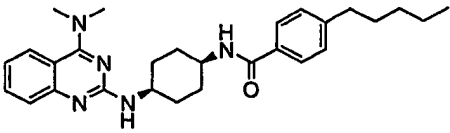
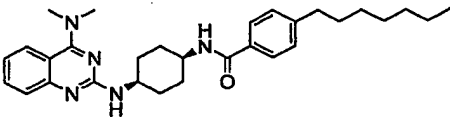
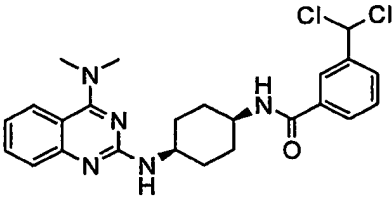
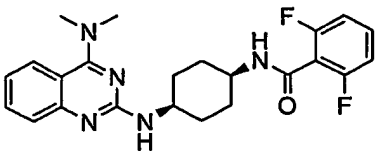
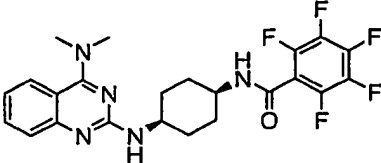
Example No.	Structure	ESI-MS	Retention Time (min)
3407	 <p>CF₃CO₂H</p>	469.4 (M + H)	4.20
3408	 <p>CF₃CO₂H</p>	436.2 (M + H)	3.88
3409	 <p>CF₃CO₂H</p>	434.4 (M + H)	3.91
3410	 <p>CF₃CO₂H</p>	558.4 (M + H)	4.92
3411	 <p>2CF₃CO₂H</p>	483.4 (M + H)	4.08
3412	 <p>CF₃CO₂H</p>	396.2 (M + H)	3.68

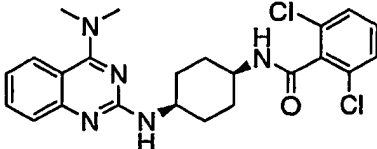
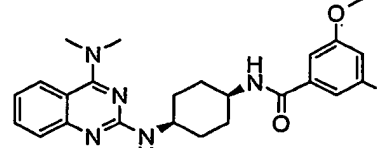
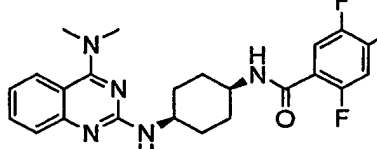
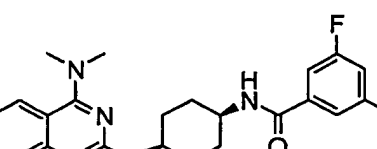
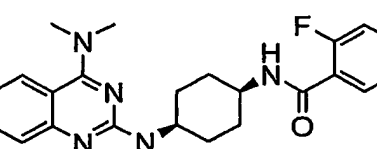
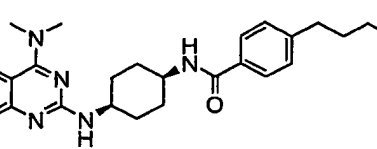
Example No.	Structure	ESI-MS	Retention Time (min)
3413	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)COc5ccc(Cl)cc5)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.70
3414	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)Cc5ccc([N+](=O)[O-])cc5C)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	449.4 (M + H)	4.09
3415	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)Cc5cc(F)c(F)c(F)c5)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.33
3416	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)c5cc(F)c(F)c(F)c5)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.60
3417	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)c5cc(F)c(F)c(F)c5)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.23
3418	 <chem>CC1(C)N2C(=NC3=CC=CC=C3N2C(=N1)N[C@H]4CCCC[C@H]4NC(=O)Cc5cc(F)c(F)c(F)c5)C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.38

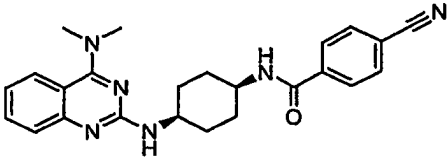
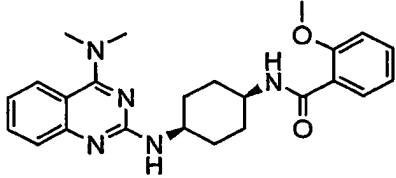
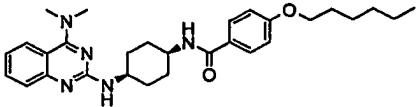
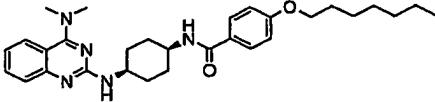
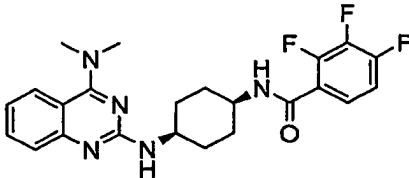
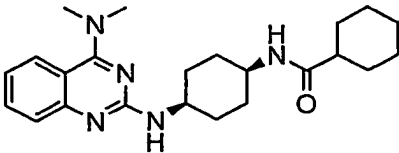
Example No.	Structure	ESI-MS	Retention Time (min)
3419	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.87
3420	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.86
3421	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.15
3422	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	4.06
3423	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc(OC)c(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	4.03
3424	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)c4cc5c(c4)OCO5</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	3.75

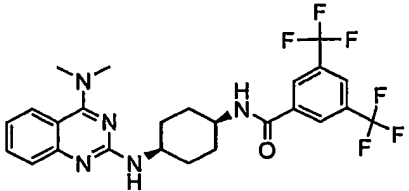
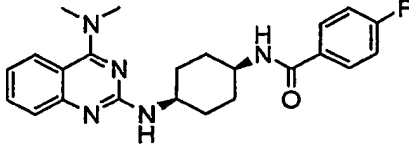
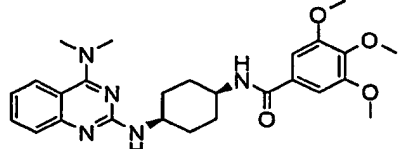
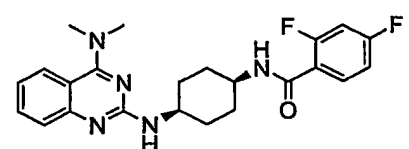
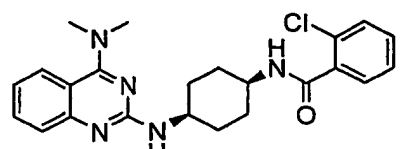
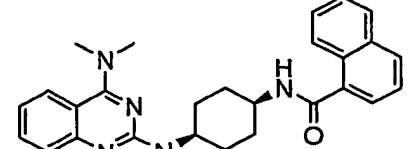
Example No.	Structure	ESI-MS	Retention Time (min)
3425	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)cc(F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.88
3426	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1cc(OC)c(OC)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.64
3427	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1cc(OC)c(O)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.55
3428	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(CC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	4.17
3429	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OCC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.03
3430	 <chem>CC1=NC2=CC=CC=C2N=CN=C1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)cc(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.45

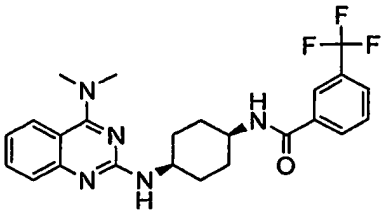
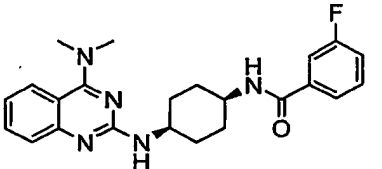
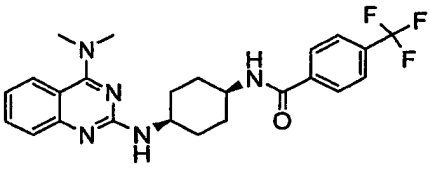
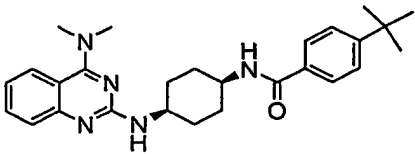
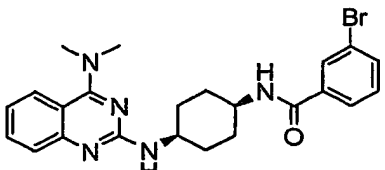
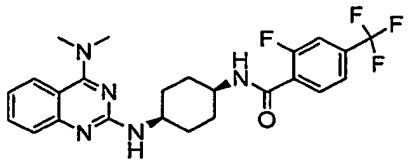
Example No.	Structure	ESI-MS	Retention Time (min)
3431	 $\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	3.76
3432	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	5.06
3433	 $\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.64
3434	 $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	4.24
3435	 $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	4.09
3436	 $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.89

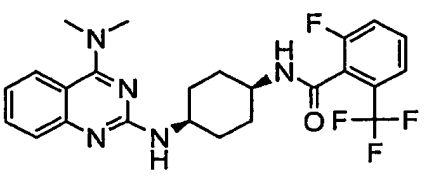
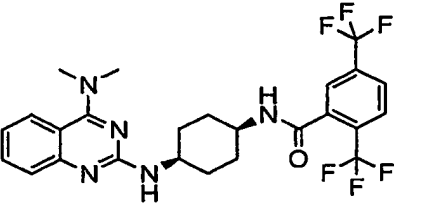
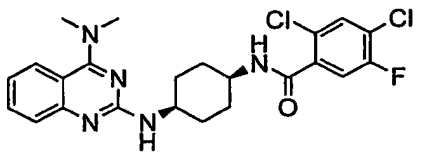
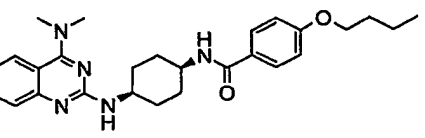
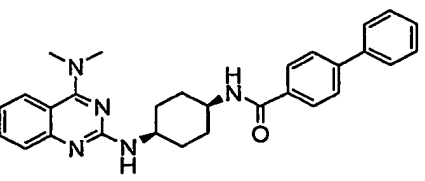
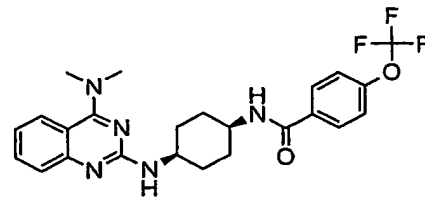
Example No.	Structure	ESI-MS	Retention Time (min)
3437	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3NC(=O)c4ccccc4I</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	3.88
3438	 <chem>CCCCCc1ccc(cc1)NC(=O)[C@H]2CCCC[C@H]2N[C@@H]3C=NC4=C(N(C)C)C=CC=C4N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	4.86
3439	 <chem>CCCCCCCCc1ccc(cc1)NC(=O)[C@H]2CCCC[C@H]2N[C@@H]3C=NC4=C(N(C)C)C=CC=C4N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	4.70
3440	 <chem>ClC(Cl)c1ccc(cc1)NC(=O)[C@H]2CCCC[C@H]2N[C@@H]3C=NC4=C(N(C)C)C=CC=C4N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.29
3441	 <chem>Fc1cc(F)ccc1NC(=O)[C@H]2CCCC[C@H]2N[C@@H]3C=NC4=C(N(C)C)C=CC=C4N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.69
3442	 <chem>Fc1c(F)c(F)c(F)cc1NC(=O)[C@H]2CCCC[C@H]2N[C@@H]3C=NC4=C(N(C)C)C=CC=C4N3</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	4.16

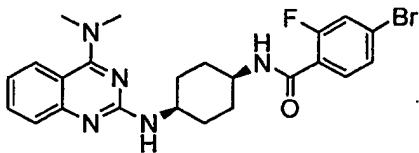
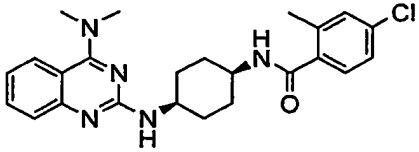
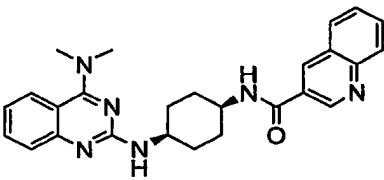
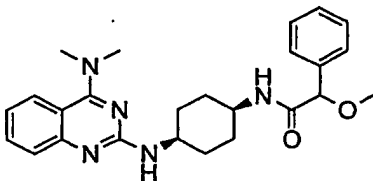
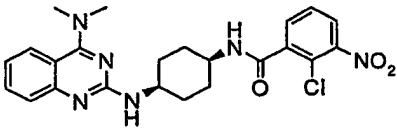
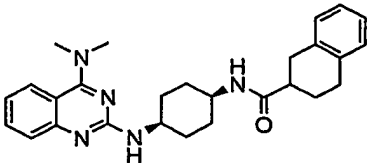
Example No.	Structure	ESI-MS	Retention Time (min)
3443	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)cc(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.91
3444	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(OC)c(OC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.95
3445	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)c(F)c(F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.01
3446	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)cc(F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	4.00
3447	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccccc1F</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	3.75
3448	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(CCC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	4.65

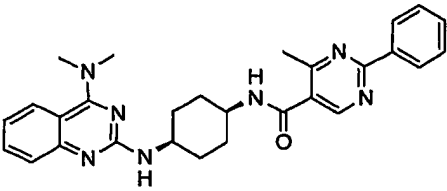
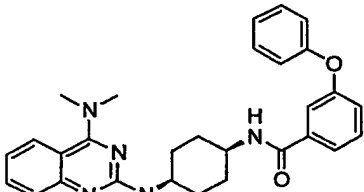
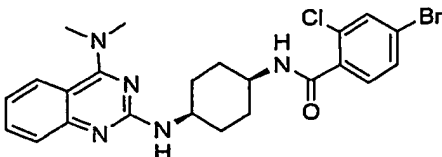
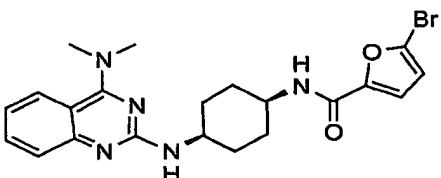
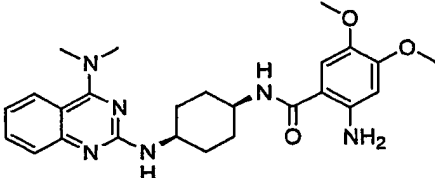
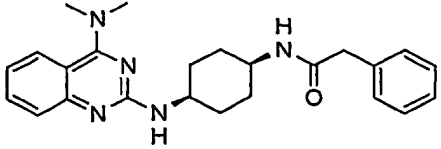
Example No.	Structure	ESI-MS	Retention Time (min)
3449	 <p>CF₃CO₂H</p>	415.2 (M + H)	3.75
3450	 <p>CF₃CO₂H</p>	420.4 (M + H)	3.91
3451	 <p>CF₃CO₂H</p>	490.4 (M + H)	4.99
3452	 <p>CF₃CO₂H</p>	504.4 (M + H)	5.16
3453	 <p>CF₃CO₂H</p>	444.4 (M + H)	4.00
3454	 <p>CF₃CO₂H</p>	396.2 (M + H)	3.85

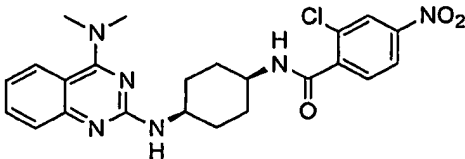
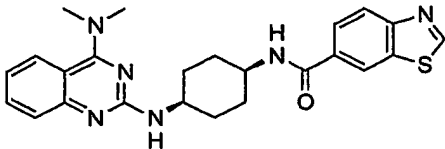
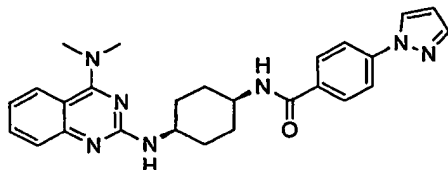
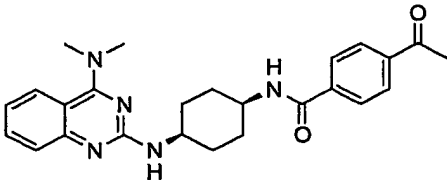
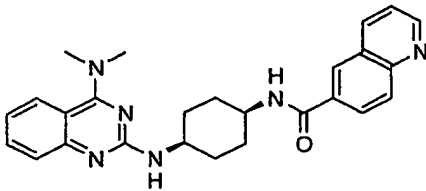
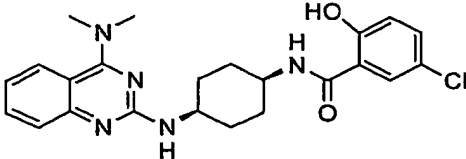
Example No.	Structure	ESI-MS	Retention Time (min)
3455	 $\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	4.69
3456	 $\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	3.30
3457	 $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	3.76
3458	 $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.86
3459	 $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.76
3460	 $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.05

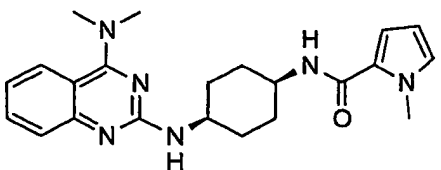
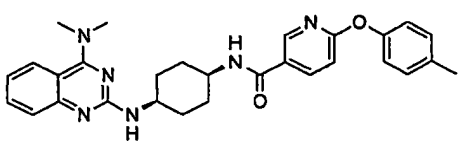
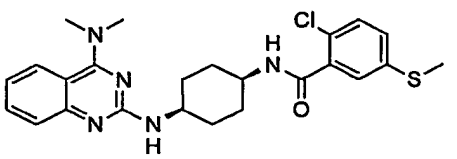
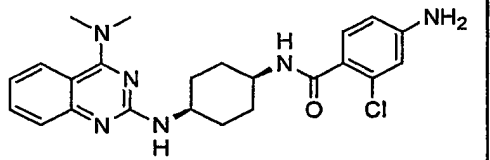
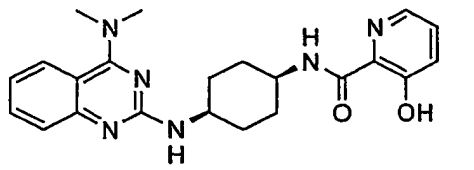
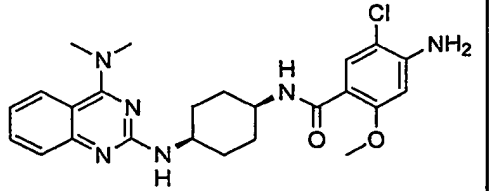
Example No.	Structure	ESI-MS	Retention Time (min)
3461	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	4.25
3462	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	3.84
3463	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.25
3464	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)C(C)(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	4.44
3465	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	4.13
3466	 <chem>CC1=NC2=CC=CC=C2N(C)N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(cc4)C(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.25

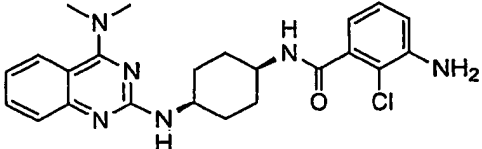
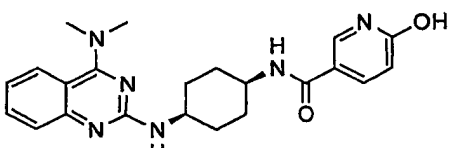
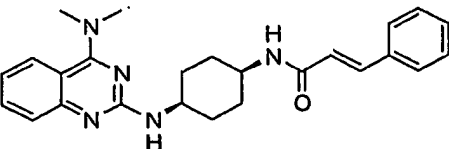
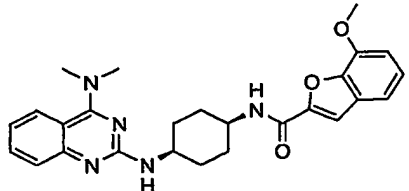
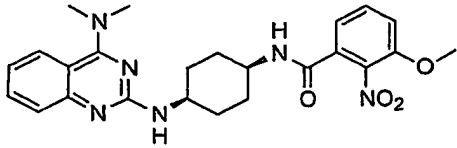
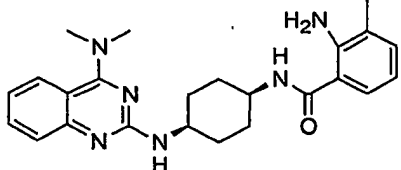
Example No.	Structure	ESI-MS	Retention Time (min)
3467	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)c(C(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.92
3468	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(C(F)(F)F)c(F)c(C(F)(F)F)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.4 (M + H)	4.31
3469	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)c(F)c(Cl)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.15
3470	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OCC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.48
3471	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(cc1)-c2ccccc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	4.45
3472	 <chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OC(F)(F)F)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.29

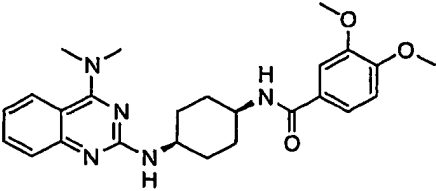
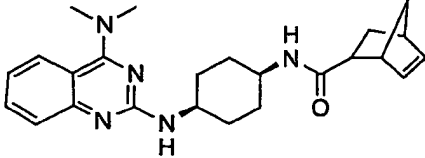
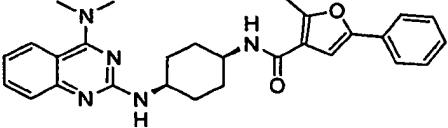
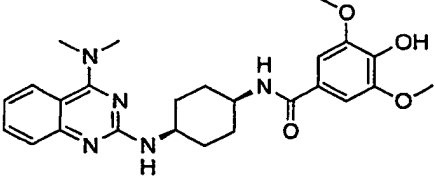
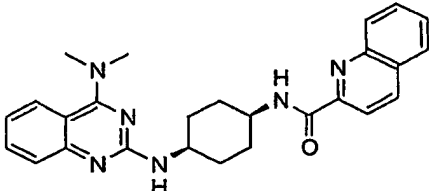
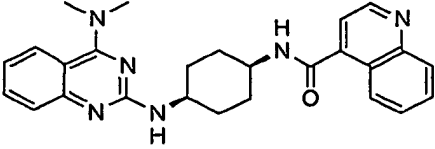
Example No.	Structure	ESI-MS	Retention Time (min)
3473	 $\text{CF}_3\text{CO}_2\text{H}$	486.2 (M + H)	4.32
3474	 $\text{CF}_3\text{CO}_2\text{H}$	438.4 (M + H)	4.31
3475	 $2\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.75
3476	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.10
3477	 $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.19
3478	 $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.36

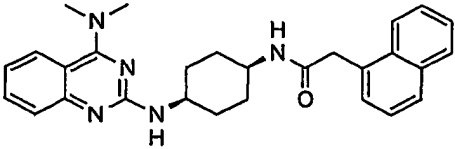
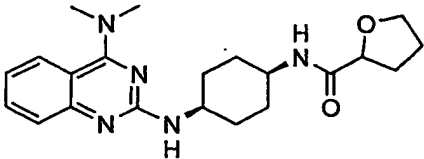
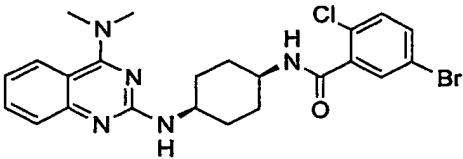
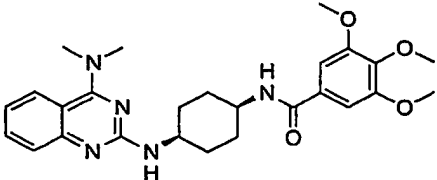
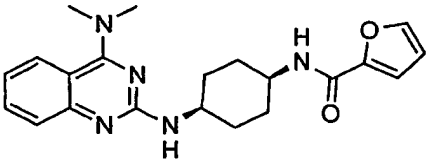
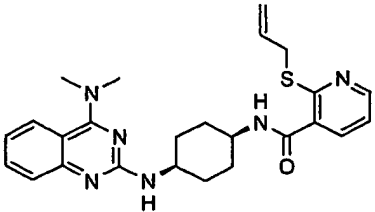
Example No.	Structure	ESI-MS	Retention Time (min)
3479	 3CF ₃ CO ₂ H	482.4 (M + H)	4.35
3480	 CF ₃ CO ₂ H	482.4 (M + H)	4.64
3481	 CF ₃ CO ₂ H	502.2 (M + H)	4.37
3482	 CF ₃ CO ₂ H	458.2 (M + H)	4.08
3483	 2CF ₃ CO ₂ H	465.4 (M + H)	3.66
3484	 CF ₃ CO ₂ H	404.4 (M + H)	4.03

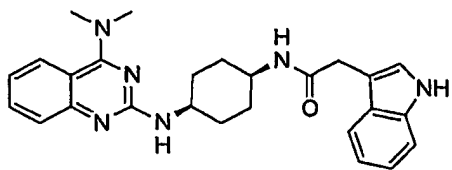
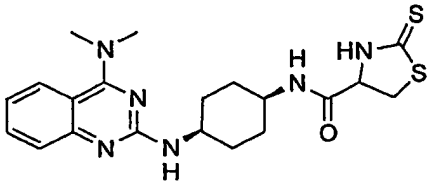
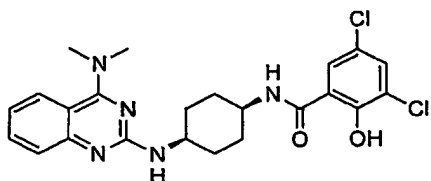
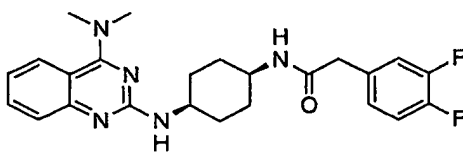
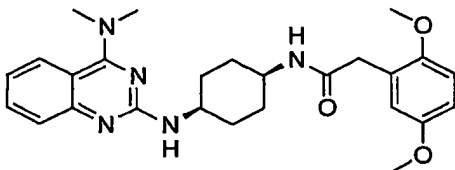
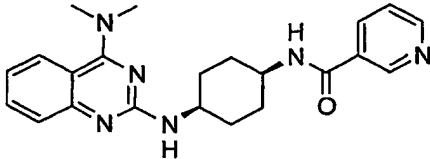
Example No.	Structure	ESI-MS	Retention Time (min)
3485	 $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.23
3486	 $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	3.94
3487	 $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	4.07
3488	 $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.99
3489	 $2\text{CF}_3\text{CO}_2\text{H}$	441.3 (M + H)	1.70
3490	 $\text{CF}_3\text{CO}_2\text{H}$	440.2 (M + H)	4.57

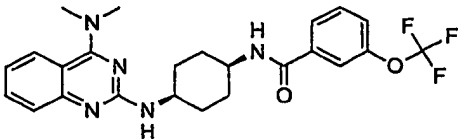
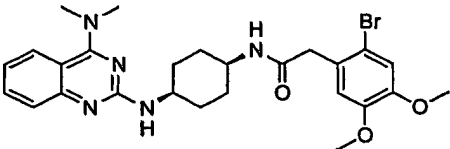
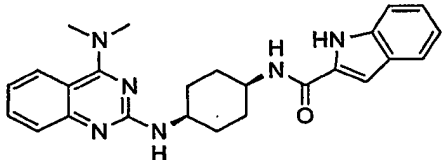
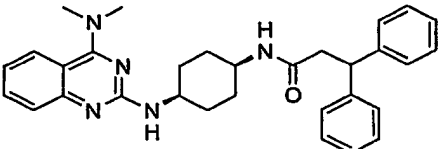
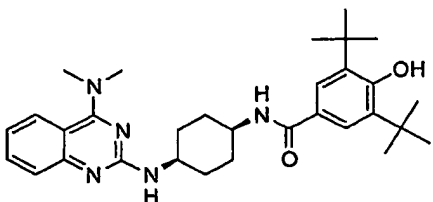
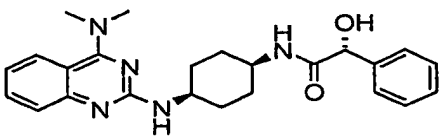
Example No.	Structure	ESI-MS	Retention Time (min)
3491	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5cc[nH]5C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	393.4 (M + H)	4.01
3492	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5ccc(oc6ccc(C)cc6)n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	4.45
3493	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5cc(Cl)cc(SC)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	2.40
3494	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5cc(N)cc(Cl)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.92
3495	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5ccc(O)c[nH]5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	2.30
3496	 <chem>CN1C=NC(=N1)N2C(=NC3=CC=CC=C3N2C)C4CCCCC4NC(=O)c5cc(N)c(Cl)c(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	469.5 (M + H)	2.27

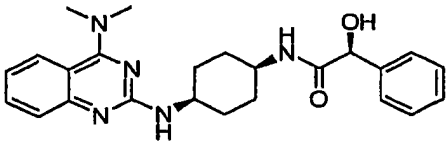
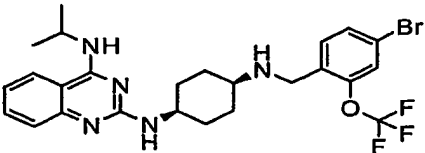
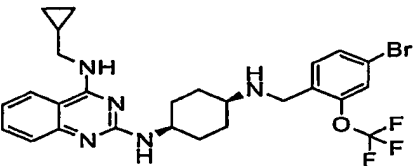
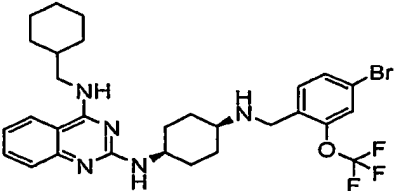
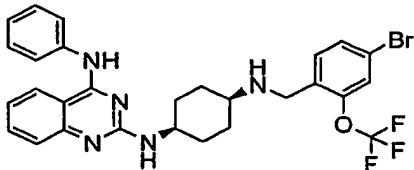
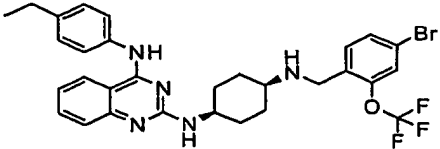
Example No.	Structure	ESI-MS	Retention Time (min)
3497	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)c3cc(N)cc(Cl)c3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.93
3498	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)c3cc(O)ccn3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	1.62
3499	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)/C=C/c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	416.3 (M + H)	2.34
3500	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)c3cc4c(cc3O4)OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	2.46
3501	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)c3ccc(OC)c([N+](=O)[O-])c3</chem> $\text{CF}_3\text{CO}_2\text{H}$	465.4 (M + H)	4.13
3502	 <chem>CC1=CN(C)C(=N1)N2CCCCC2NC(=O)c3cc(N)c(C)cc3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	3.87

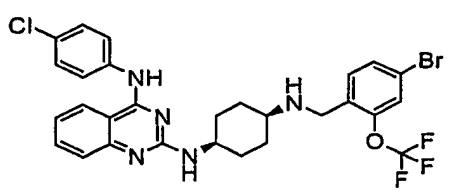
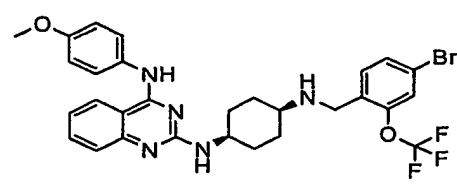
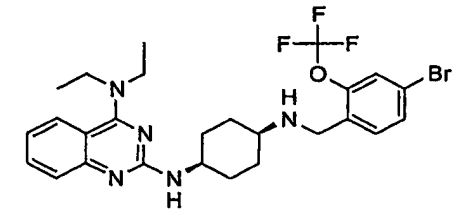
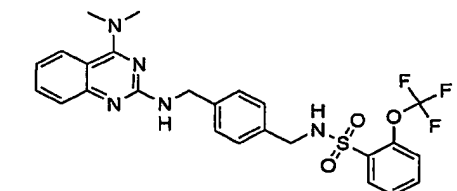
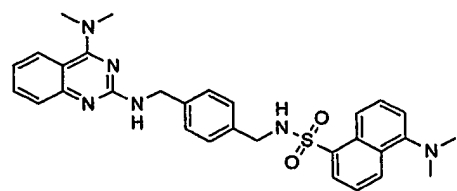
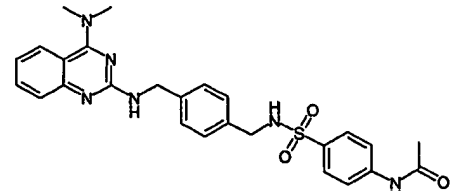
Example No.	Structure	ESI-MS	Retention Time (min)
3503	 $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.97
3504	 $\text{CF}_3\text{CO}_2\text{H}$	406.2 (M + H)	2.18
3505	 $\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	4.74
3506	 $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.83
3507	 $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	4.38
3508	 $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	3.62

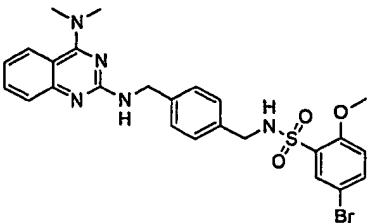
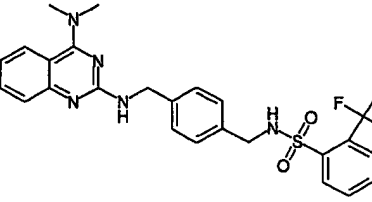
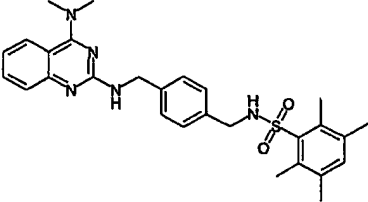
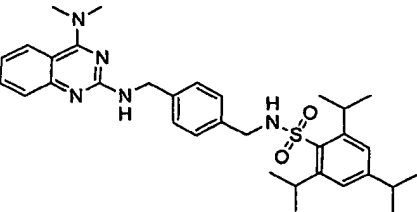
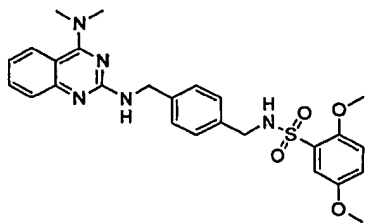
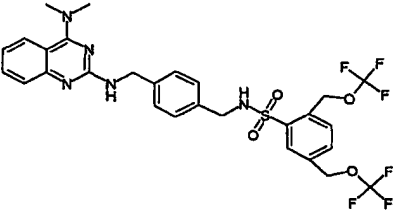
Example No.	Structure	ESI-MS	Retention Time (min)
3509	 $\text{CF}_3\text{CO}_2\text{H}$	454.5 (M + H)	2.44
3510	 $\text{CF}_3\text{CO}_2\text{H}$	384.4 (M + H)	3.67
3511	 $\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	4.37
3512	 $\text{CF}_3\text{CO}_2\text{H}$	480.5 (M + H)	2.18
3513	 $\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	3.81
3514	 $2\text{CF}_3\text{CO}_2\text{H}$	463.2 (M + H)	4.23

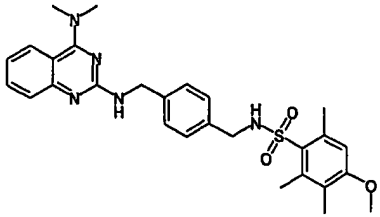
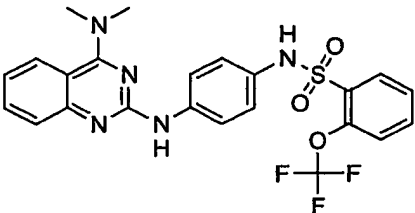
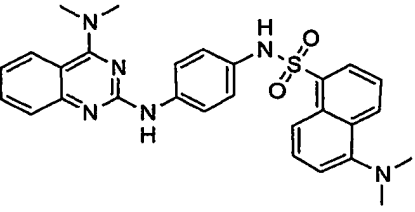
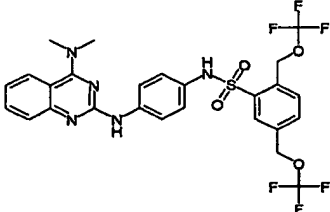
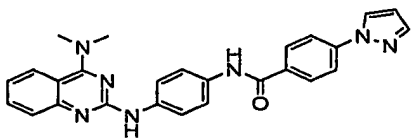
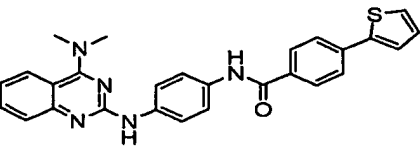
Example No.	Structure	ESI-MS	Retention Time (min)
3515	 $2\text{CF}_3\text{CO}_2\text{H}$	443.4 (M + H)	2.12
3516	 $\text{CF}_3\text{CO}_2\text{H}$	431.1 (M + H)	1.90
3517	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	5.05
3518	 $\text{CF}_3\text{CO}_2\text{H}$	440.5 (M + H)	2.33
3519	 $\text{CF}_3\text{CO}_2\text{H}$	464.5 (M + H)	2.20
3520	 $2\text{CF}_3\text{CO}_2\text{H}$	391.1 (M + H)	1.59

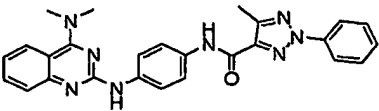
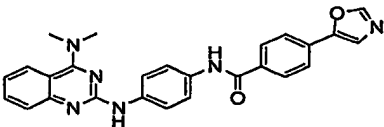
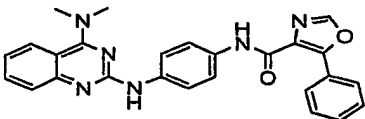
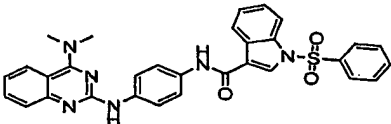
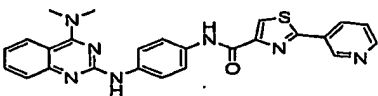
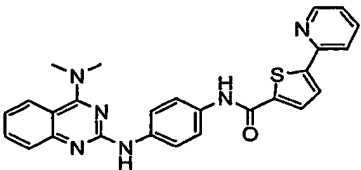
Example No.	Structure	ESI-MS	Retention Time (min)
3521	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.53
3522	 $\text{CF}_3\text{CO}_2\text{H}$	542.2 (M + H)	2.26
3523	 $2\text{CF}_3\text{CO}_2\text{H}$	429.3 (M + H)	2.41
3524	 $\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.59
3525	 $\text{CF}_3\text{CO}_2\text{H}$	518.5 (M + H)	2.96
3526	 $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.19

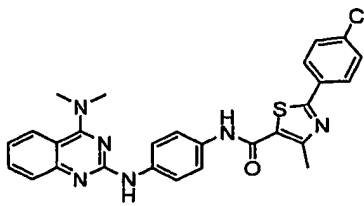
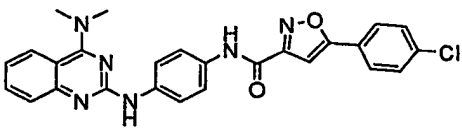
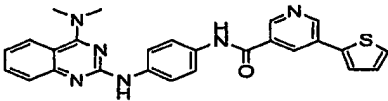
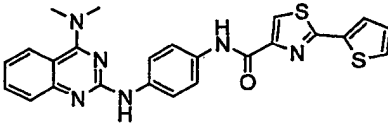
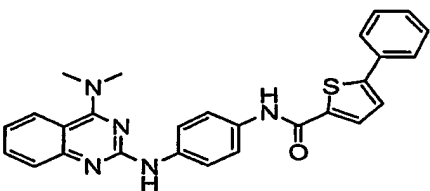
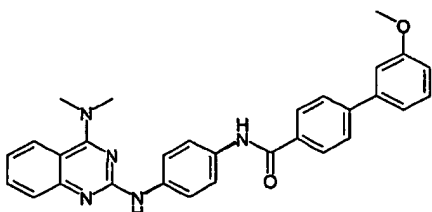
Example No.	Structure	ESI-MS	Retention Time (min)
3527	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)C(O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.19
3528	 <chem>CC(C)Nc1nc2ccccc2n1C(=N)N[C@H]3CCCC[C@H]3NC(=O)Cc4ccc(Br)c(OC(F)(F)F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	2.45
3529	 <chem>C1CC1CNc2nc3ccccc3n2C(=N)N[C@H]4CCCC[C@H]4NC(=O)Cc5ccc(Br)c(OC(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	564.2 (M + H)	2.48
3530	 <chem>C1CCCCC1CNc2nc3ccccc3n2C(=N)N[C@H]4CCCC[C@H]4NC(=O)Cc5ccc(Br)c(OC(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	606.0 (M + H)	2.86
3531	 <chem>c1ccc(cc1)CNc2nc3ccccc3n2C(=N)N[C@H]4CCCC[C@H]4NC(=O)Cc5ccc(Br)c(OC(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	3.20
3532	 <chem>CCc1ccc(cc1)CNc2nc3ccccc3n2C(=N)N[C@H]4CCCC[C@H]4NC(=O)Cc5ccc(Br)c(OC(F)(F)F)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	614.4 (M + H)	2.76

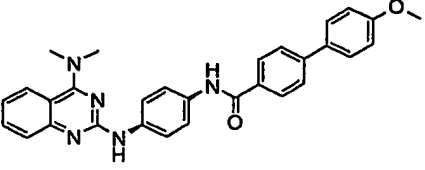
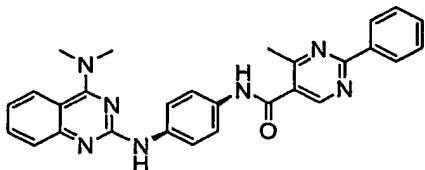
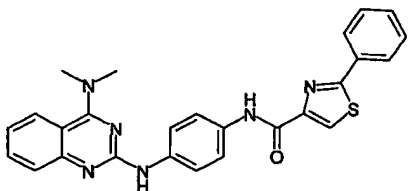
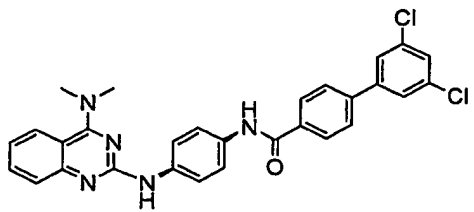
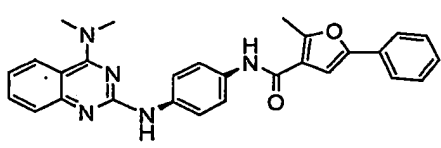
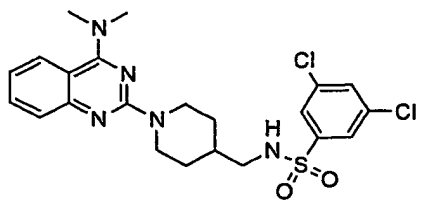
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3533	 $2\text{CF}_3\text{CO}_2\text{H}$	620.0 (M + H)	2.68
3534	 $2\text{CF}_3\text{CO}_2\text{H}$	616.0 (M + H)	2.56
3535	 $2\text{CF}_3\text{CO}_2\text{H}$	566.0 (M + H)	2.54
3536	 $\text{CF}_3\text{CO}_2\text{H}$	532.2 (M + H)	3.35
3537	 $2\text{CF}_3\text{CO}_2\text{H}$	541.4 (M + H)	3.11
3538	 $\text{CF}_3\text{CO}_2\text{H}$	505.2 (M + H)	2.98

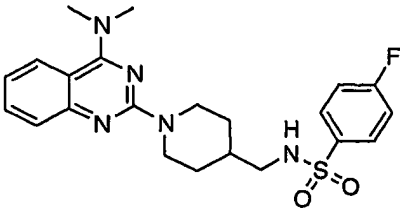
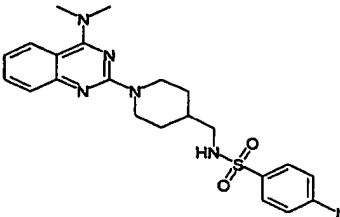
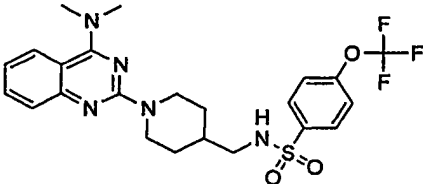
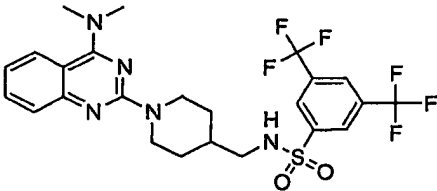
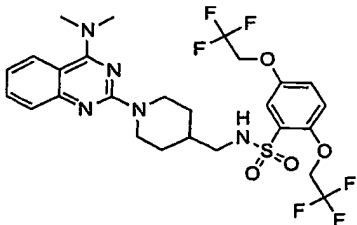
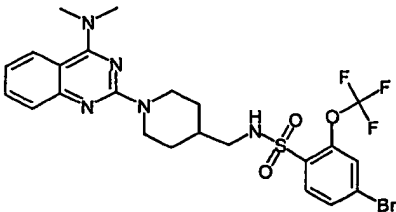
Example No.	Structure	ESI-MS	Retention Time (min)
3539	 <chem>COc1cc(Br)cc(S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	556 (M + H)	3.37
3540	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.39
3541	 <chem>Cc1cc(C)cc(C)cc1S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	3.61
3542	 <chem>Cc1cc(C)cc(C)cc1S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	574.4 (M + H)	4.27
3543	 <chem>COc1cc(OC)cc(S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.17
3544	 <chem>COc1cc(OC(F)(F)F)cc(S(=O)(=O)NCc2ccc(cc2)Nc3nc4ccccc4n3C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	3.63

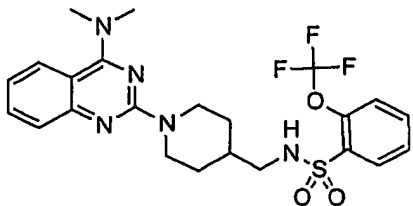
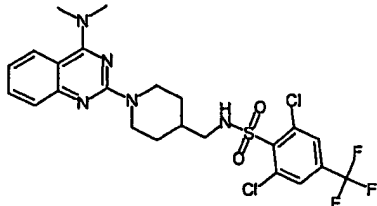
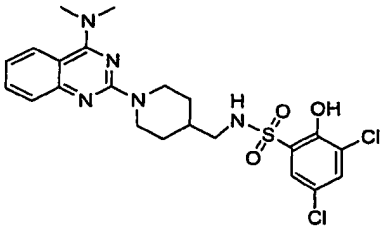
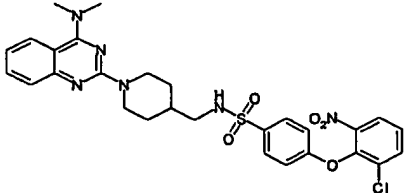
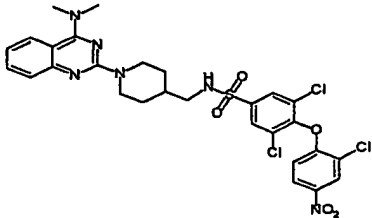
Example No.	Structure	ESI-MS	Retention Time (min)
3545	 $\text{CF}_3\text{CO}_2\text{H}$	520.4 (M + H)	3.56
3546	 $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.25
3547	 $2\text{CF}_3\text{CO}_2\text{H}$	513.4 (M + H)	2.86
3548	 $\text{CF}_3\text{CO}_2\text{H}$	616.2 (M + H)	3.73
3549	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.79
3550	 $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.35

Example No.	Structure	ESI-MS	Retention Time (min)
3551	 $2\text{CF}_3\text{CO}_2\text{H}$	465.2 (M + H)	3.34
3552	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	3.83
3553	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	4.10
3554	 $\text{CF}_3\text{CO}_2\text{H}$	563.2 (M + H)	4.33
3555	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.66
3556	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	2.85

Example No.	Structure	ESI-MS	Retention Time (min)
3557	 $\text{CF}_3\text{CO}_2\text{H}$	515.4 (M + H)	3.52
3558	 $\text{CF}_3\text{CO}_2\text{H}$	485.2 (M + H)	3.40
3559	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.90
3560	 $\text{CF}_3\text{CO}_2\text{H}$	473.4 (M + H)	4.17
3561	 $\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.57
3562	 $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	4.00

Example No.	Structure	ESI-MS	Retention Time (min)
3563	 <chem>COc1ccc(cc1)C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.99
3564	 <chem>c1cc2nc(NC3=CC=CC=C3)nc(C2=O)n1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.76
3565	 <chem>c1cc2nc(NC3=CC=CC=C3)nc(C2=O)n1</chem> $\text{CF}_3\text{CO}_2\text{H}$	467.2 (M + H)	4.07
3566	 <chem>Clc1cc(Cl)ccc1C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	4.53
3567	 <chem>c1cc2oc(NC3=CC=CC=C3)cc(C2=O)n1</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	4.11
3568	 <chem>Clc1cc(Cl)ccc1NS(=O)(=O)CC2CCN(C2)c3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.0 (M + H)	3.43

Example No.	Structure	ESI-MS	Retention Time (min)
3569	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.0 (M + H)	3.03
3570	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4ccc(I)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.30
3571	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.37
3572	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4ccc(C(F)(F)F)cc4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.66
3573	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4cc(OC(F)(F)F)cc(OC(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	622.0 (M + H)	3.61
3574	 <chem>CC1=NC2=CC=CC=C2N(C)N=C1CN3CCCCC3CNS(=O)(=O)c4cc(OC(F)(F)F)cc(Br)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	588.0 (M + H)	3.59

Example No.	Structure	ESI-MS	Retention Time (min)
3575	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccccc4OC(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.31
3576	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(Cl)c(Cl)cc4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.61
3577	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(Cl)c(Cl)c(O)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.35
3578	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(Oc5cc(Cl)ccc5)cc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	597.0 (M + H)	3.55
3579	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(Cl)c(Oc5cc(Cl)cc([N+](=O)[O-])cc5)cc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	665.0 (M + H)	4.02

Assay Procedures

Compounds identified and disclosed throughout this patent document were assayed according to the protocols found in co-pending patent application having U.S. Serial Number 09/826,509, which is incorporated herein by reference.

Example 3580

Preparation of Endogenous MCH Receptor.

The endogenous human MCH receptor was obtained by PCR using genomic DNA as template and rTth polymerase (Perkin Elmer) with the buffer system provided by the manufacturer, 0.25 μ M of each primer, and 0.2 mM of each 4 nucleotides. The cycle condition was 30 cycles of 94°C for 1 min, 56°C for 1min and 72 °C for 1 min and 20 sec. The 5' PCR primer contained a HindIII site with the sequence:

5'-GTGAAGCTTGCCTCTGGTGCCTGCAGGAGG-3' (SEQ.ID.NO.:1)

and the 3' primer contained an EcoRI site with the sequence:

5'-GCAGAATTCCCGGTGGCGTGTTGTGGTGCCC-3' (SEQ.ID.NO.:2).

The 1.3 kb PCR fragment was digested with HindIII and EcoRI and cloned into HindIII-EcoRI site of CMVp expression vector. Later the cloning work by Lakaye et al showed that there is an intron the coding region of the gene. Thus the 5' end of the cDNA was obtained by 5' RACE PCR using Clontech's marathon-ready hypothalamus cDNA as template and the manufacturer's recommended protocol for cycling condition. The 5' RACE PCR for the first and second round PCR were as follows:

5'-CATGAGCTGGTGGATCATGAAGGG-3' (SEQ.ID.NO.:3) and

5'-ATGAAGGGCATGCCAGGAGAAAG-3' (SEQ.ID.NO.:4).

Nucleic acid and amino acid sequences were thereafter determined and verified with the published sequences found on GenBank having Accession Number U71092.

Example 3581

Preparation of Non-Endogenous, Constitutively Active MCH Receptor.

Preparation of a non-endogenous version of the human MCH receptor was accomplished by creating a MCH-IC3-SST2 mutation (*see*; SEQ.ID.NO.:7 for nucleic acid sequence, and SEQ.ID.NO.:8 for amino acid sequence). Blast result showed that MCH receptor had the highest sequence homology to known SST2 receptor. Thus the third intracellular loop ("IC3") of MCH receptor was replaced with that of the IC3 of SST2

receptor to see if the chimera would show constitutive activity.

The BamHI-BstEII fragment containing IC3 of MCH receptor was replaced with synthetic oligonucleotides that contained the IC3 of SST2. The PCR sense mutagenesis primer used had the following sequence:

5'-GATCCTGCAGAAGGTGAAGTCCTCTGGAATCCGAGTGGGCTCCTCTAAGAG
GAAGAAGTCTGAGAAGAAG-3' (SEQ.ID.NO.:9)

and the antisense primer had the following sequence:

5'-GTGACCTTCTTCTCAGACTTCTTCCTCTTAGAGGAGCCCACTCGGATTCCAG
AGGACTTCACCTTCTGCAG-3' (SEQ.ID.NO.:10).

The endogenous MCH receptor cDNA was used as a template.

Example 3582

GPCR Fusion Protein Preparation.

MCH Receptor-Gi α Fusion Protein construct was made as follows: primers were designed for endogenous MCH receptor was as follows:

5'-GTGAAGCTTGCCCGGGCAGGATGGACCTGG-3' (SEQ.ID.NO.:11; sense)

5'-ATCTAGAGGTGCCTTTGCTTTCTG-3' (SEQ.ID.NO.:12; anitsense).

The sense and anti-sense primers included the restriction sites for KB4 and XbaI, respectively.

PCR was utilized to secure the respective receptor sequences for fusion within the Gi α universal vector disclosed above, using the following protocol for each: 100ng cDNA for MCH receptor was added to separate tubes containing 2ul of each primer (sense and anti-sense), 3uL of 10mM dNTPs, 10uL of 10XTaqPlus™ Precision buffer, 1uL of TaqPlus™ Precision polymerase (Stratagene: #600211), and 80uL of water. Reaction temperatures and cycle times for MCH receptor were as follows: the initial denaturing step was done it 94°C for five minutes, and a cycle of 94°C for 30 seconds; 55°C for 30 seconds; 72°C for two minutes. A final extension time was done at 72°C for ten minutes. PCR product for was run on a 1% agarose gel and then purified (data not shown). The purified product was digested with KB4 and XbaI (New England Biolabs) and the desired inserts will be isolated, purified and ligated into the Gi universal vector at the respective restriction site. The positive clones was isolated following transformation and determined by restriction enzyme digest; expression using 293 cells was accomplished

following the protocol set forth *infra*. Each positive clone for MCH receptor: Gi-Fusion Protein was sequenced and made available for the direct identification of candidate compounds. (See, SEQ.ID.NO.:13 for nucleic acid sequence and SEQ.ID.NO.:14 for amino acid sequence).

Endogenous version of MCH receptor was fused upstream from the G protein Gi and is located at nucleotide 1 through 1,059 (see, SEQ.ID.NO.:13) and amino acid residue 1 through 353 (see, SEQ.ID.NO.:14). With respect to the MCH receptor, 2 amino acid residues (an equivalent of 6 nucleotides) were placed in between the endogenous (or non-endogenous) GPCR and the start codon for the G protein $G_{i\alpha}$. Therefore, the Gi protein is located at nucleotide 1,066 through 2,133 (see, SEQ.ID.NO.:13) and at amino acid residue 356 through 711 (see, SEQ.ID.NO.:14). Those skilled in the art are credited with the ability to select techniques for constructing a GPCR Fusion Protein where the G protein is fused to the 3' end of the GPCR of interest.

Example 3583

ASSAY FOR DETERMINATION OF CONSTITUTIVE ACTIVITY OF NON-ENDOGENOUS GPCRS

A. Intracellular IP_3 Accumulation Assay

On day 1, cells comprising the receptors (endogenous and/or non-endogenous) can be plated onto 24 well plates, usually 1×10^5 cells/well (although this number can be optimized). On day 2 cells can be transfected by firstly mixing 0.25 μ g DNA in 50 μ l serum free DMEM/well and 2 μ l lipofectamine in 50 μ l serum-free DMEM/well. The solutions are gently mixed and incubated for 15-30 min at room temperature. Cells are washed with 0.5 ml PBS and 400 μ l of serum free media is mixed with the transfection media and added to the cells. The cells are then incubated for 3-4 hrs at $37^\circ\text{C}/5\%\text{CO}_2$ and then the transfection media is removed and replaced with 1ml/well of regular growth media. On day 3 the cells are labeled with ^3H -myo-inositol. Briefly, the media is removed and the cells are washed with 0.5 ml PBS. Then 0.5 ml inositol-free/serum free media (GIBCO BRL) is added/well with 0.25 μCi of ^3H -myo-inositol/ well and the cells are incubated for 16-18 hrs o/n at $37^\circ\text{C}/5\%\text{CO}_2$. On Day 4 the cells are washed with 0.5 ml PBS and 0.45 ml of assay medium is added containing inositol-free/serum free media 10 μM pargyline 10 mM lithium chloride or 0.4 ml of assay medium and 50 μ l of $10 \times$

ketanserin (ket) to final concentration of 10 μ M. The cells are then incubated for 30 min at 37°C. The cells are then washed with 0.5 ml PBS and 200 μ l of fresh/ice cold stop solution (1M KOH; 18 mM Na-borate; 3.8 mM EDTA) is added/well. The solution is kept on ice for 5-10 min or until cells were lysed and then neutralized by 200 μ l of fresh/ice cold neutralization sol. (7.5 % HCL). The lysate is then transferred into 1.5 ml eppendorf tubes and 1 ml of chloroform/methanol (1:2) is added/tube. The solution is vortexed for 15 sec and the upper phase is applied to a Biorad AG1-X8™ anion exchange resin (100-200 mesh). Firstly, the resin is washed with water at 1:1.25 W/V and 0.9 ml of upper phase is loaded onto the column. The column is washed with 10 mls of 5 mM myo-inositol and 10 ml of 5 mM Na-borate/60mM Na-formate. The inositol tris phosphates are eluted into scintillation vials containing 10 ml of scintillation cocktail with 2 ml of 0.1 M formic acid/ 1 M ammonium formate. The columns are regenerated by washing with 10 ml of 0.1 M formic acid/3M ammonium formate and rinsed twice with H₂O and stored at 4°C in water.

Reference is made to Figure 1. Figure 1 provides an illustration of IP₃ production from several non-endogenous, constitutively activated version of MCH receptor as compared with the endogenous version of this receptor. When compared to the endogenous version of MCH receptor ("MCH-R wt"), MCH-IC3-SST2 evidenced about a 27% increase in IP₃ accumulation.

Example 3584

Determination of Compound Using [³⁵S]GTP γ S ASSAY

Direct identification of candidate compounds was initially screened using [³⁵S]GTP γ S Assay (see, Example 6 of co-pending patent application 09/826,509). Preferably, an MCH receptor: Gi Fusion Protein was utilized, according to Example 6(2) of co-pending patent application 09/826,509. Several lead hits were identified utilizing [³⁵S]GTP γ S Assay.

Example 3585

High Throughput Functional Screening: FLIPR™

Subsequently, a functional based assay was used to confirm the lead hits, referred to as FLIPR™ (the Fluorometric Imaging Plate Reader) and FDSS6000™ (Functional

Drug Screening System). This assay utilized a non-endogenous version of the MCH receptor, which was created by swapping the third intracellular loop of the MCH receptor with that of the SST2 receptor (see Example 2(B)(2) of patent application serial number 09/826,509).

The FLIPR and FDSS assays are able to detect intracellular Ca^{2+} concentration in cells, which can be utilized to assess receptor activation and determine whether a candidate compound is an, for example, antagonist, inverse agonist or agonist to a Gq-coupled receptor. The concentration of free Ca^{2+} in the cytosol of any cell is extremely low, whereas its concentration in the extracellular fluid and endoplasmic reticulum (ER) is very high. Thus, there is a large gradient tending to drive Ca^{2+} into the cytosol across both the plasma membrane and ER. The FLIPRTM and FDSS6000TM systems (Molecular Devices Corporation, HAMAMATSU Photonics K.K.) are designed to perform functional cell-based assays, such as the measurement of intracellular calcium for high-throughput screening. The measurement of fluorescent is associated with calcium release upon activation of the Gq-coupled receptors. Gi or Go coupled receptors are not as easily monitored through the FLIPRTM and FDSS6000TM systems because these G proteins do not couple with calcium signal pathways.

To confirm the lead hits identified using the [³⁵S]GTPγS assay, Fluorometric Imaging Plate Reader system was used to allow for rapid, kinetic measurements of intracellular fluorescence in 96 well microplates (or 384 well microplates). Simultaneous measurements of fluorescence in all wells can be made by FLIPR or FDSS6000TM every second with high sensitivity and precision. These systems are ideal for measuring cell-based functional assays such as monitoring the intracellular calcium fluxes that occur within seconds after activation of the Gq coupled receptor.

Briefly, the cells are seeded into 96 well at 5.5×10^4 cells/well with complete culture media (Dulbecco's Modified Eagle Medium with 10 % fetal bovine serum, 2 mM L-glutamine, 1 mM sodium pyruvate and 0.5 mg/ml G418, pH 7.4) for the assay next day. On the day of assay, the media is removed and the cells are incubated with 100 μl of loading buffer (4 μM Fluo4-AM in complete culture media containing 2.5 mM Probenicid, 0.5 mg/ml and 0.2% bovine serum albumin) in 5% CO₂ incubator at 37°C for 1 hr. The loading buffer is removed, and the cells are washed with wash buffer (Hank's Balanced Salt Solution containing 2.5 mM Probenicid, 20 mM HEPES, 0.5 mg/ml and 0.2% bovine

serum albumin, pH 7.4)). One hundred fifty μ l of wash buffer containing various concentrations of test compound are added to the cells, and the cells are incubated in 5% CO₂ incubator at 37°C for 30 min. Fifty μ l of wash buffer containing various concentration of MCH are added to each well, and transient changes in [Ca²⁺]_i evoked by MCH are monitored using the FLIPR or FDSS in 96 well plates at Ex. 488 nm and Em. 530 nm for 290 second. When antagonist activity of compound is tested, 50 nM of MCH is used.

Use of FLIPR™ and FDSS6000™ can be accomplished by following manufacturer's instruction (Molecular Device Corporation and HAMAMATSU Photonics K.K.).

The results were shpwn below.

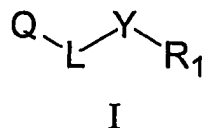
Compound No.	IC ₅₀ value (nM)
Example 41	6
Example 42	19

It is intended that each of the patents, applications, printed publications, and other published documents mentioned or referred to in this specification be herein incorporated by reference in their entirety.

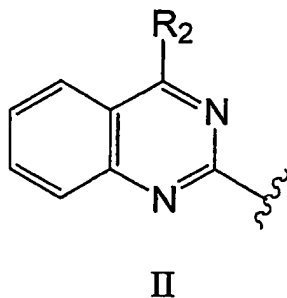
Those skilled in the art will appreciate that numerous changes and modifications may be made to the preferred embodiments of the invention and that such changes and modifications may be made without departing from the spirit of the invention. It is therefore intended that the appended claims cover all such equivalent variations as fall within the true spirit and scope of the invention.

What is claimed is:

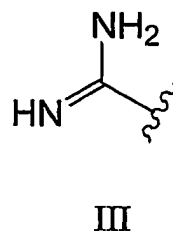
1. A compound of Formula I:



wherein Q is



or



R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

- halogen,
- hydroxy,
- oxo,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by substituent(s) independently selected from
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by C₁-C₃ alkyl,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
- halogen,
- nitro,
- carbocyclic aryl,
- carbocyclic aryl substituted by C₁-C₃ alkoxy,

- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
- oxo,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
- carbocyclic arylcarbonylamino,
- halogenated carbocyclic arylcarbonylamino,
- heterocycloxy,
- heterocycloxy substituted by C₁-C₃ alkyl,
- substituted heterocyclyl-ethylideneaminoxy,
- C₁-C₃ alkoxy carbonyl,
- C₁-C₃ alkoxy carbonyl substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
- cyano,
- carbocyclic aryl,
- heterocyclyl,
- mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
- hydroxy,
- C₁-C₃ alkyl,
- C₁-C₃ alkylcarbonylamino,
- C₁-C₃ alkylcarbonylamino substituted by substituent(s) independently selected from
- C₁-C₃ alkylcarbonylamino,
- carbocyclic arylcarbonylamino,
- heterocyclyl,
- C₁-C₄ alkoxy carbonylamino,
- heterocyclyl carbonylamino,
- carbocyclic arylsulfonylamino,

- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - C₃-C₆ cycloalkenyl,
 - carbocyclyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₂-C₃ alkenyl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
- C₁-C₄ alkoxy,
- C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-carbocyclic arylamino,

- halogenated mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - mercapto,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,

- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
- heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- (iii) C₂-C₄ alkynyl,
 - C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - carbocyclic arylcarbonylamino,
 - carbocyclic aryl,
- (v) C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
- (vi) carbocyclyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - hydroxy,

- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,

- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- C₂-C₃ alkenyloxy,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - halogenated C₁-C₄ alkyl,
 - C₁-C₃ alkoxy,
 - heterocyclyloxy,
 - heterocyclyloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,

- carboxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkynylcarbonylamino,
- C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- carbocyclic aryl diazo,
- carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - cyano,
 - C₁-C₃ alkyl,
 - heterocyclylthio,
 - C₁-C₃ alkylsulfonyl,
 - mono- or di-C₁-C₃ alkylaminosulfonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocyclic arylcarbonylamino,
 - halogenated carbocyclic arylcarbonylamino,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₄ alkylcarbonylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - halogenated carbocyclic arylthio,
 - carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - C₁-C₃ alkoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,

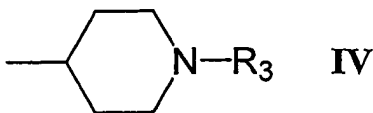
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy carbonyl;

R₂ is -NHNH₂, -NHNHBoc, -N(R_{2a})(R_{2b}), morpholino, 4-acetyl-piperazyl, or 4-phenyl-piperazyl;

wherein R_{2a} is H or C₁-C₃ alkyl;

R_{2b} is C₁-C₄ alkyl, C₁-C₄ alkyl substituted by substituent(s) independently selected from

- hydroxy,
 - C₁-C₃ alkoxy,
 - amino,
 - NHBoc,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - SO₂NH₂,
 - heterocyclyl,
- C₃-C₆ cycloalkyl, carbocyclic aryl, carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- or a group of Formula IV;

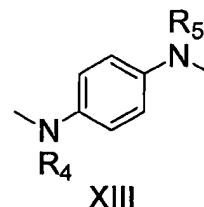
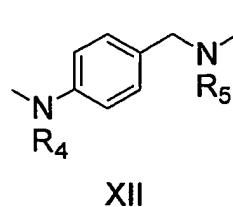
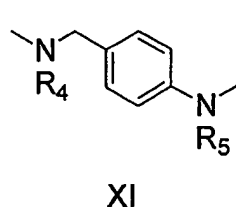
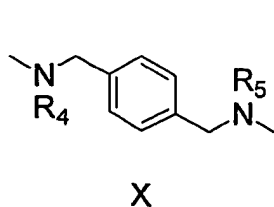
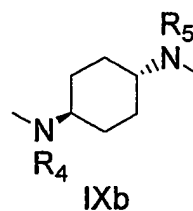
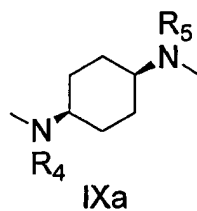
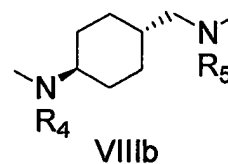
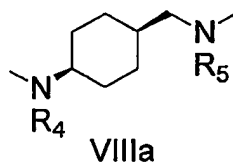
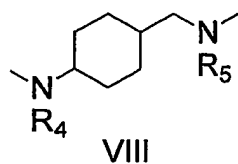
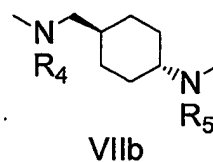
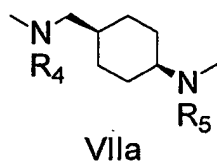
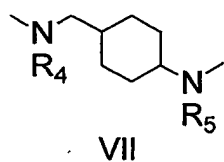
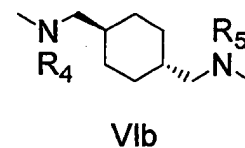
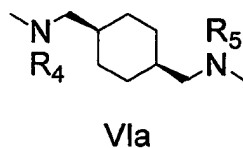
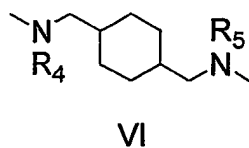
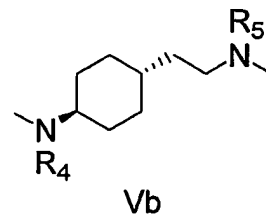
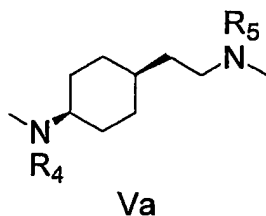
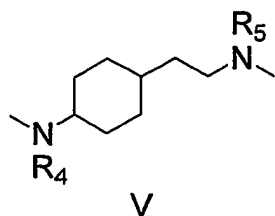


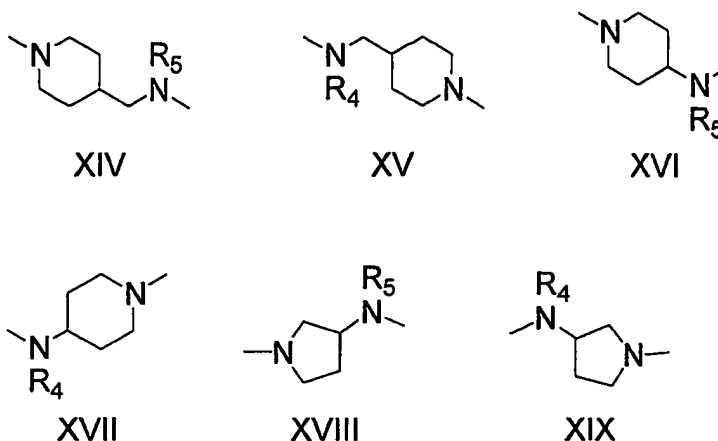
wherein Boc is carbamic acid *tert*-butyl ester and R₃ is C₁-C₃ alkyl or C₁-C₃ alkyl

substituted by substituent(s) independently selected from

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by C₁-C₃ alkoxy;

L is selected from Formula V - XIX;





wherein R_4 is H or C_1 - C_3 alkyl;

R_5 is H, C_1 - C_3 alkyl, or C_1 - C_3 alkyl substituted by a substituted carbocyclic aryl;

Y is $-S(O)_2-$, $-C(O)-$, or $-(CH_2)_m$;

m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, biphenyl, or phenanthryl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolo[2,3-c]pyridyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4H-benzo[1,3]dioxinyl, 4H-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-carbazolyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, benzofuryl, benzothiazolyl, cinnolyl, furyl, imidazo[2,1-b]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperazyl, piperidyl, piridyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-

dihydro-benzofuryl, tetrahydro-thienyl, or benzofuranyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

2. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

•halogen,

•oxo,

•C₁-C₃ alkoxy,

•C₁-C₃ alkoxy substituted by carbocyclic aryl,

•C₁-C₃ alkylcarbonyloxy,

•carbocycloxy,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C₁-C₄ alkyl,

••C₁-C₄ alkyl substituted by substituent(s) independently selected from

•••oxo,

•••carbocyclic arylcarbonylamino,

•••halogenated carbocyclic arylcarbonylamino,

•heterocycloxy,

•heterocycloxy substituted by C₁-C₃ alkyl,

•substituted heterocyclyl-ethylideneaminoxy,

•C₁-C₃ alkoxycarbonyl,

•C₁-C₃ alkoxycarbonyl substituted by carbocyclic aryl,

•mono- or di-C₁-C₃ alkylaminocarbonyl,

•mono- or di-carbocyclic arylamino,

•mono- or di-carbocyclic arylamino substituted by hydroxy,

•C₁-C₃ alkylcarbonylamino,

- C₁-C₃ alkylcalbonylamino substituted by substituent(s) independently selected from
 - C₁-C₃ alkylcalbonylamino,
 - carbocyclic arylcalbonylamino,
 - heterocyclyl,
- C₁-C₄ alkoxycalbonylamino,
- heterocyclyl calbonylamino,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - C₃-C₆ cycloalkenyl,

- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,

- C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - mercapto,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₆ alkenyl,
- C₂-C₆ alkenyl substituted by substituent(s) independently selected from
- oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,

- C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- (iii) C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - carbocyclic arylcarbonylamino,
 - carbocyclic aryl,
- (iv) carbocyclyl,
- carbocyclyl substituted by nitro,
- (v) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryloxy,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,

- heterocyclyl,
- heterocyclyl substituted by C₁-C₃ alkyl,
- C₁-C₇ alkoxy,
- C₁-C₇ alkoxy substituted by substituent(s) independently selected from
- halogen,
- carbocyclic aryl,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
- amino,
- mono- or di-C₁-C₃ alkylamino,
- C₁-C₃ alkynylcarbonylamino,
- C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by cyano,
- C₁-C₃ alkylsulfonyl,
- mono- or di-C₁-C₃ alkylaminosulfonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (vi) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,

- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -C(O)-;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isindolyl, 1H-indolyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, cinnolyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

3. A compound according to claim 2, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
 - C₅-C₆ cycloalkyl,
 - C₅-C₆ cycloalkenyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from

- oxo,
- carbocyclic aryl,
- heterocyclyl,
- C₁-C₄ alkoxy,
- halogenated C₁-C₄ alkoxy,
- C₁-C₄ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated mono-carbocyclic arylaminocarbonyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C₁-C₂ alkyl,
- C₁-C₂ substituted by carbocyclic aryl,
- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
- methyl substituted by oxo,
- methyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- hydroxy,

- cyano,
- nitro,
- C₁-C₉ alkyl,
- C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₇ alkoxy,
 - halogenated C₁-C₇ alkoxy,
 - C₁-C₇ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,
 - mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - heterocyclyl substituted by methyl,
 - heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,

- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein R₄ and R₅ are independently selected from H or C₁-C₃ alkyl;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isoindolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, azetidyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl,

quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, cinnolyl, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;
or a salt thereof.

4. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
- C₅-C₆ cycloalkenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,

- ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - halogenated C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,

(iv) carbocyclyl,

(v) carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,

- hydroxy,

- cyano,

- nitro,

- C₁-C₉ alkyl,

- C₁-C₉ alkyl substituted by substituent(s) independently selected from

- halogen,

- oxo,

- carbocyclic aryl,

- carbocyclic aryl substituted by methyl,

- carbocyclic aryloxy,

- C₁-C₇ alkoxy,

- halogenated C₁-C₇ alkoxy,

- C₁-C₇ alkoxy substituted by carbocyclic aryl,

- methylcarbonyloxy,

- carbocyclic aryloxy,

- carbocyclic aryloxy substituted by methoxy,

- amino,

- di-methylamino,

- propargynylcarbonylamino substituted by carbocyclic aryl,

- carbocyclic arylsulfonylamino substituted by methyl,

- (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,

- halogenated methylthio,

- carbocyclic arylthio substituted by cyano,

- di-propylamino sulfonyl,

- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,

- carbocyclic aryl,

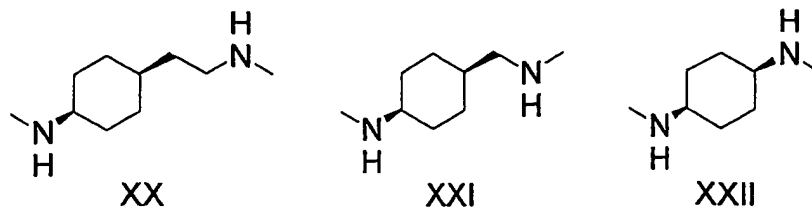
- heterocyclyl substituted by methyl,

- heterocyclyl substituted by halogenated carbocyclic aryl,

(vi) or heterocyclyl substituted by substituent(s) independently selected from

- halogen,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
- methoxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by methyl,
- C₁-C₃ alkylthio,
- propenylthio,
- carbocyclic arylthio,
- C₁-C₃ alkylsulfonyl,
- carbocyclic arylsulfonyl,
- carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methyl,
- carbocyclic aryl substituted by nitro,
- heterocyclyl;

L is selected from Formula XX - XXII;



wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-

9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 4-oxo-benzopyranyl, azetidiny, benzo[b]thienyl, furyl, isoxazolyl, morpholinyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 9*H*-xanthenyl, cinnolyl, imidazolyl, morpholino, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

5. A compound according to claim 4, wherein

R₁ represents

(i) C₁-C₅ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminooxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methoxy,
- carbocyclic arylthio,
- heterocyclylthio substituted by nitro,
- heterocyclylthio substituted by methyl,

- cyclohexenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,

- carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₂ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,

- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by methyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, indenyl, 9-oxo-fluorenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

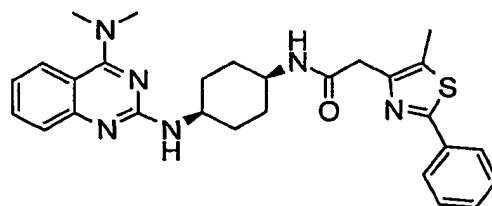
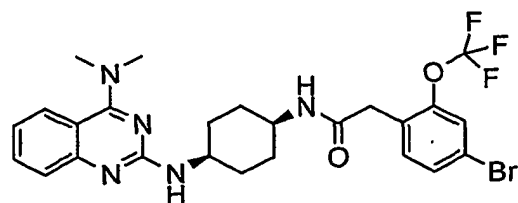
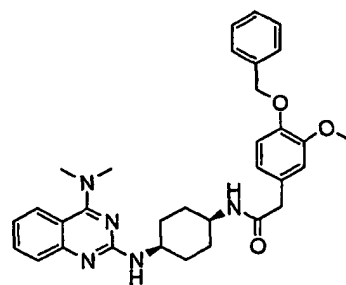
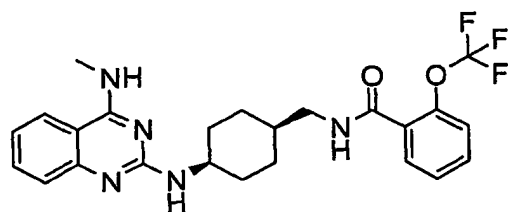
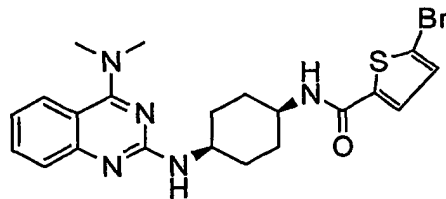
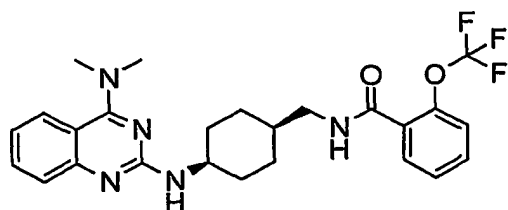
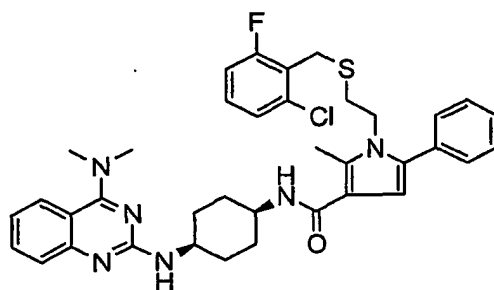
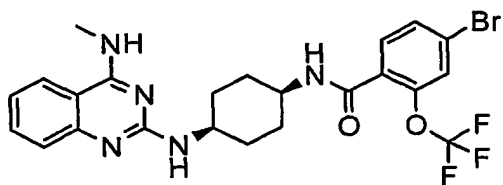
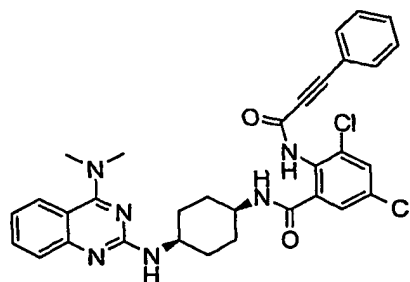
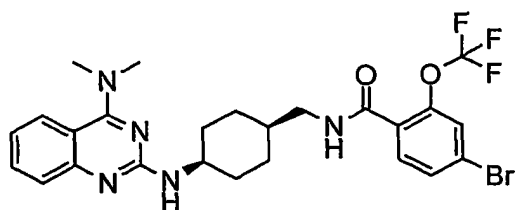
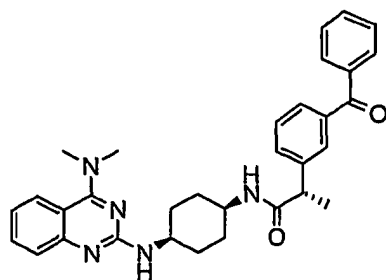
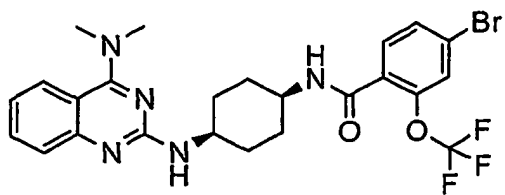
heterocyclyl is 1*H*-indolyl, 2,4-dihydro-3-oxo-pyrazolyl, furyl, pyrazolyl, pyridyl,

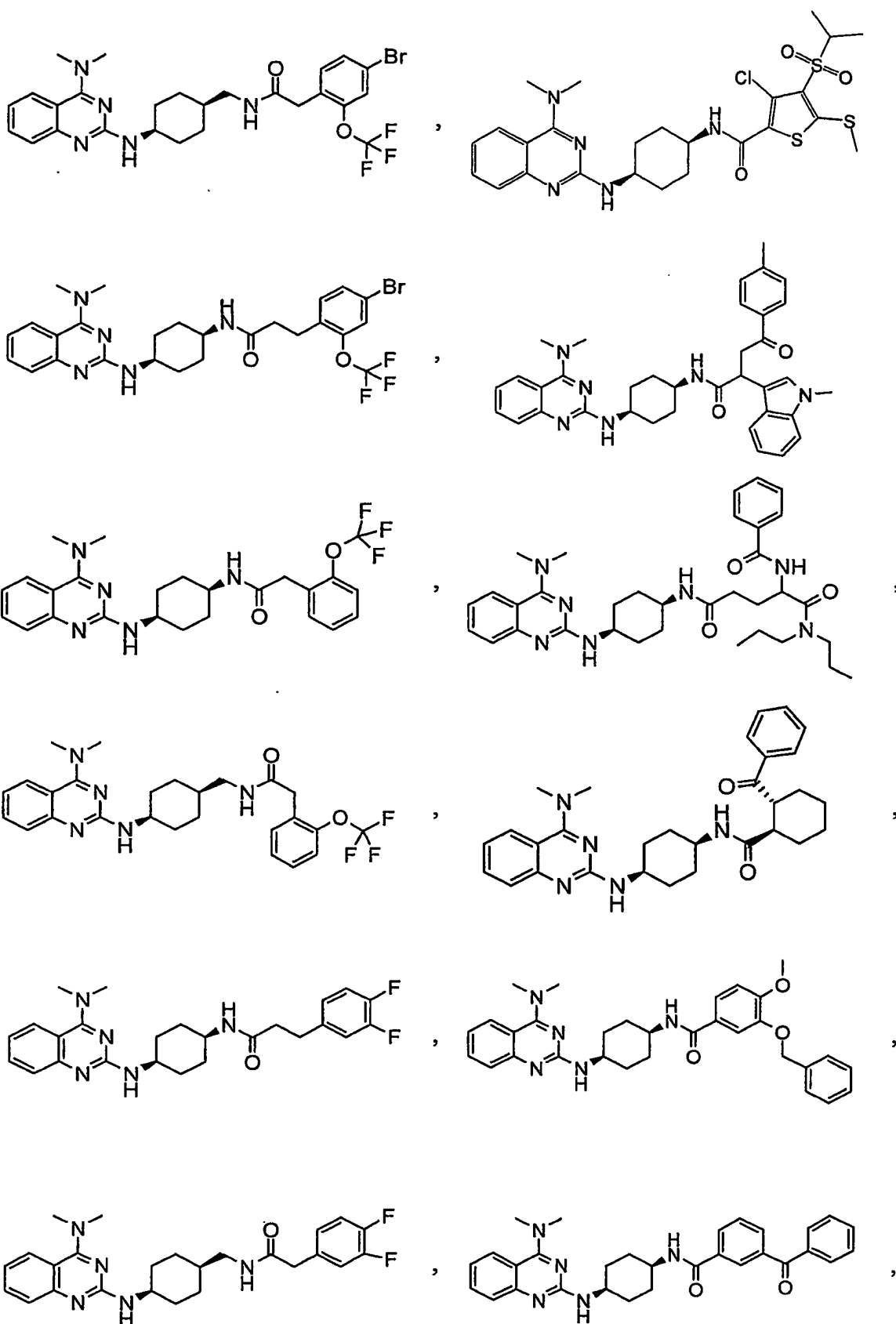
thienyl, 1,2,3-triazolyl, 1*H*-pyrrolyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, pyrazolyl, pyrimidyl, quinolyl, thiazolyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

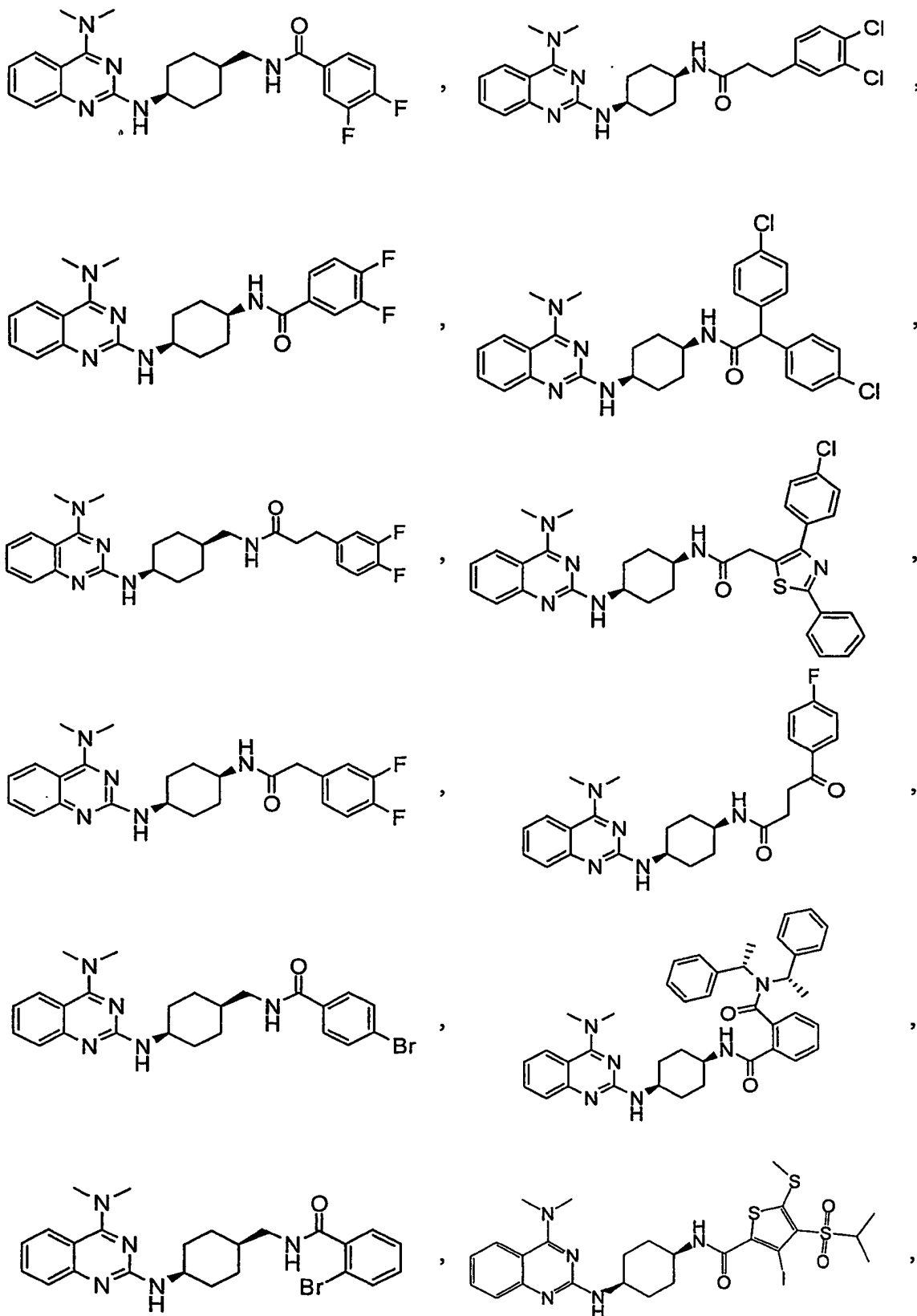
halogen is fluoro, chloro, bromo, or iodo;

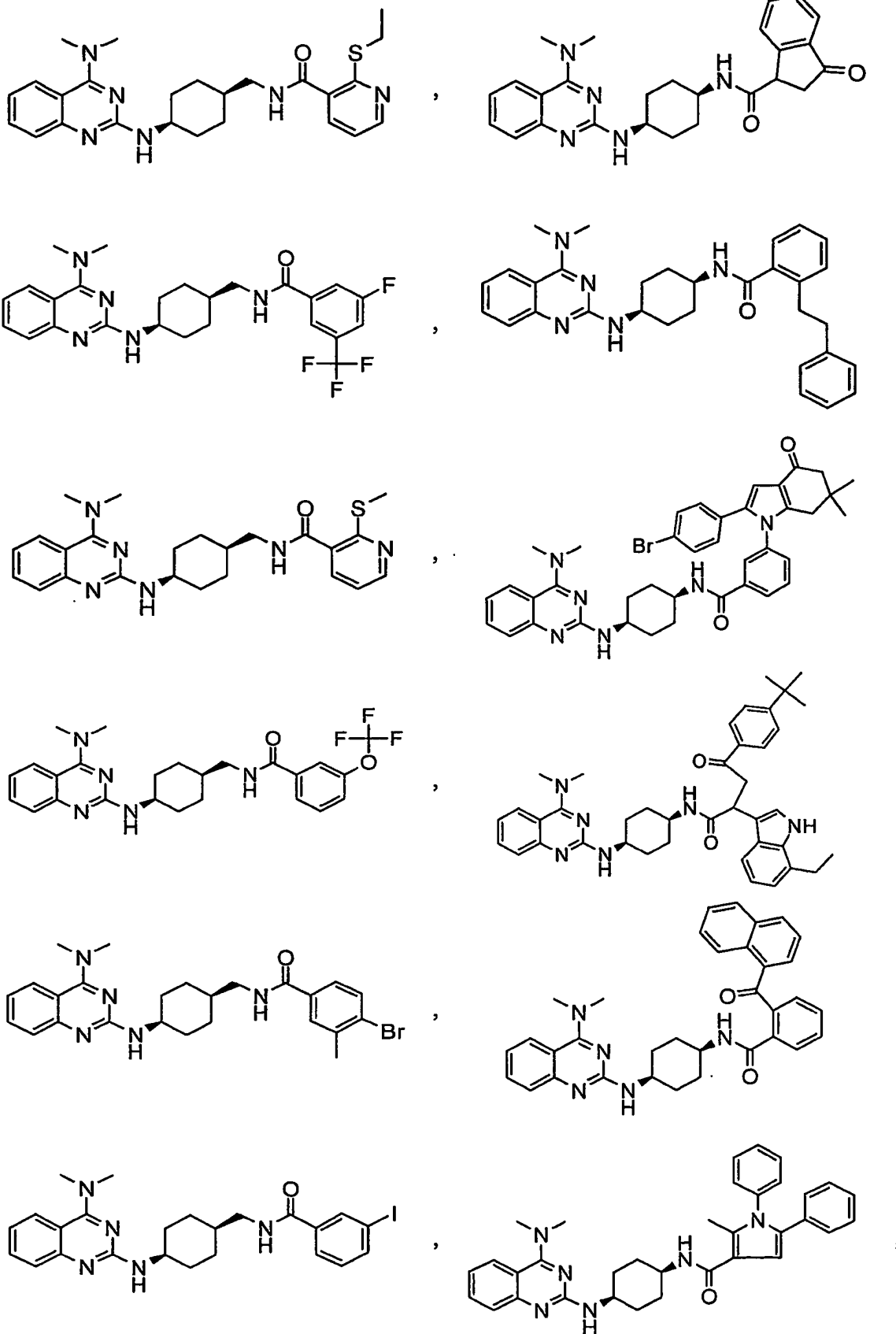
or a salt thereof.

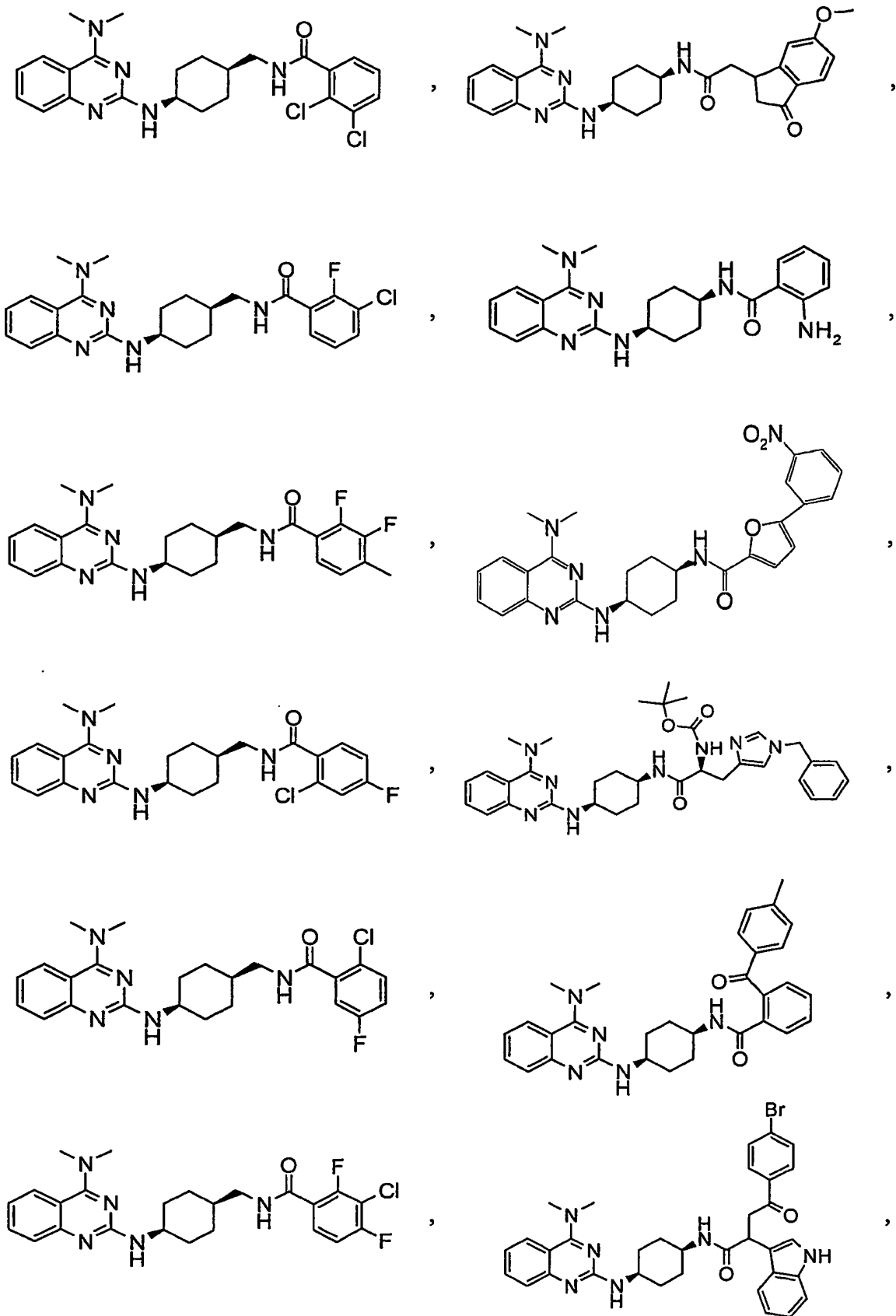
6. A compound according to claim 5 of Formula I selected from the group consisting of

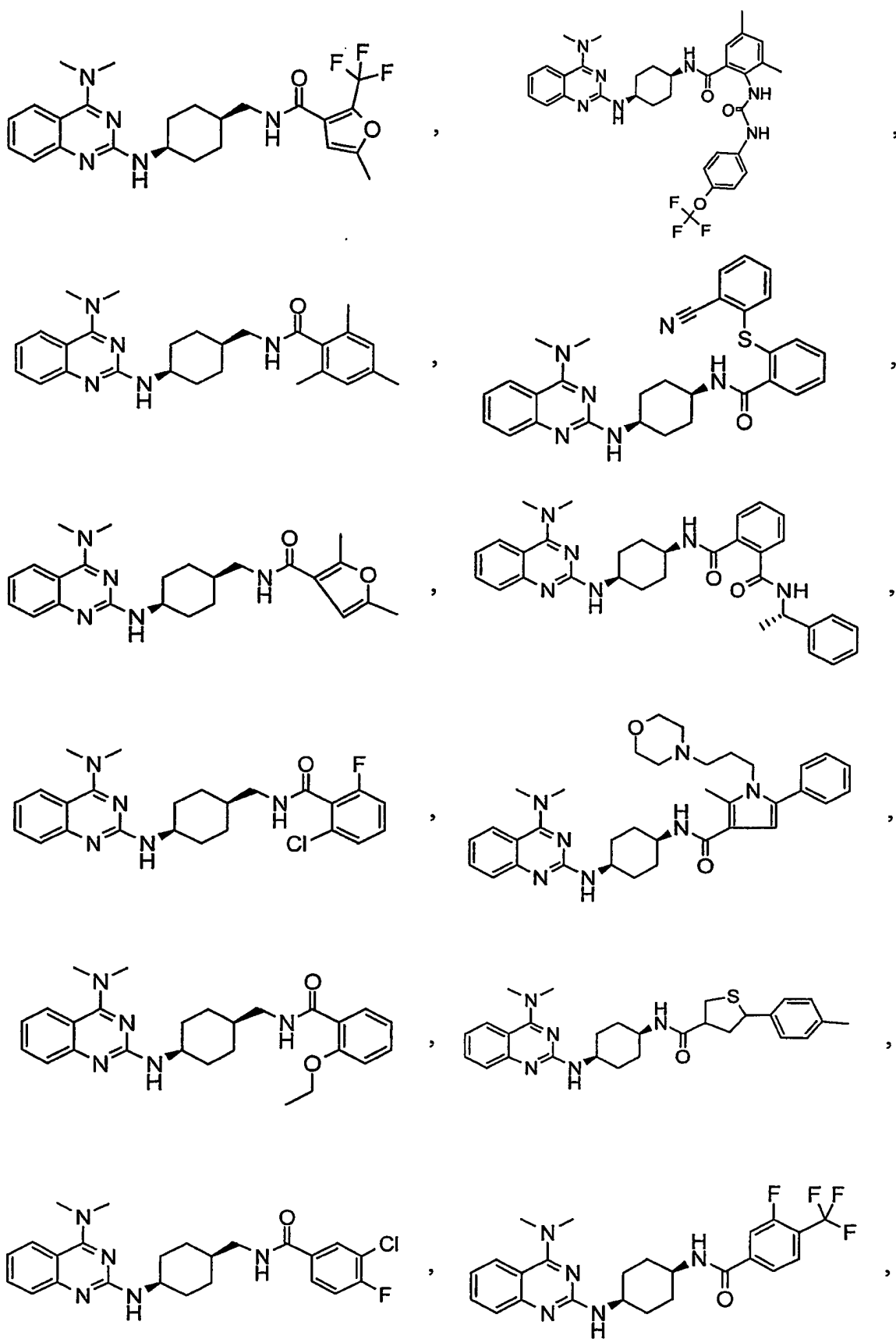


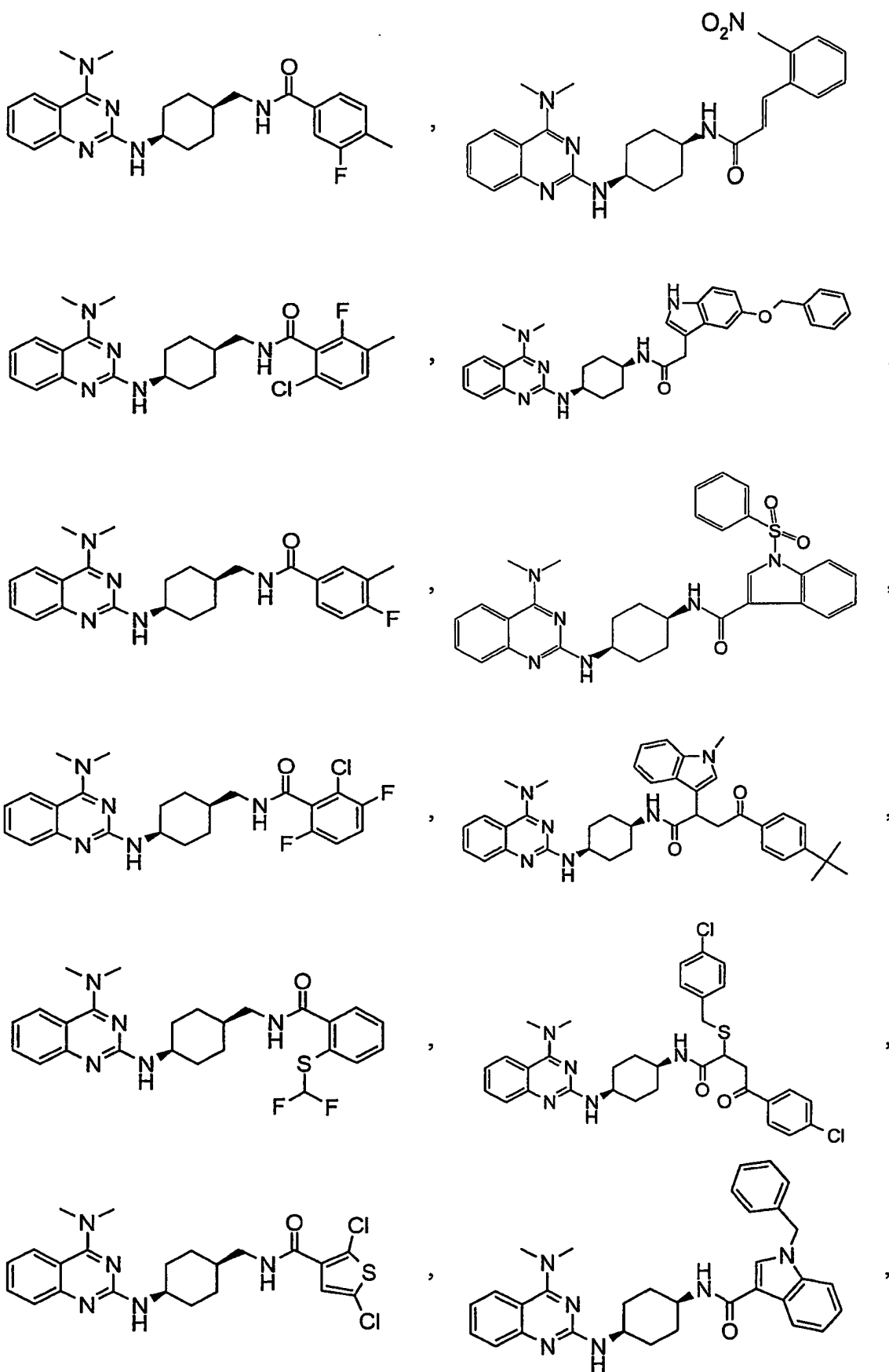


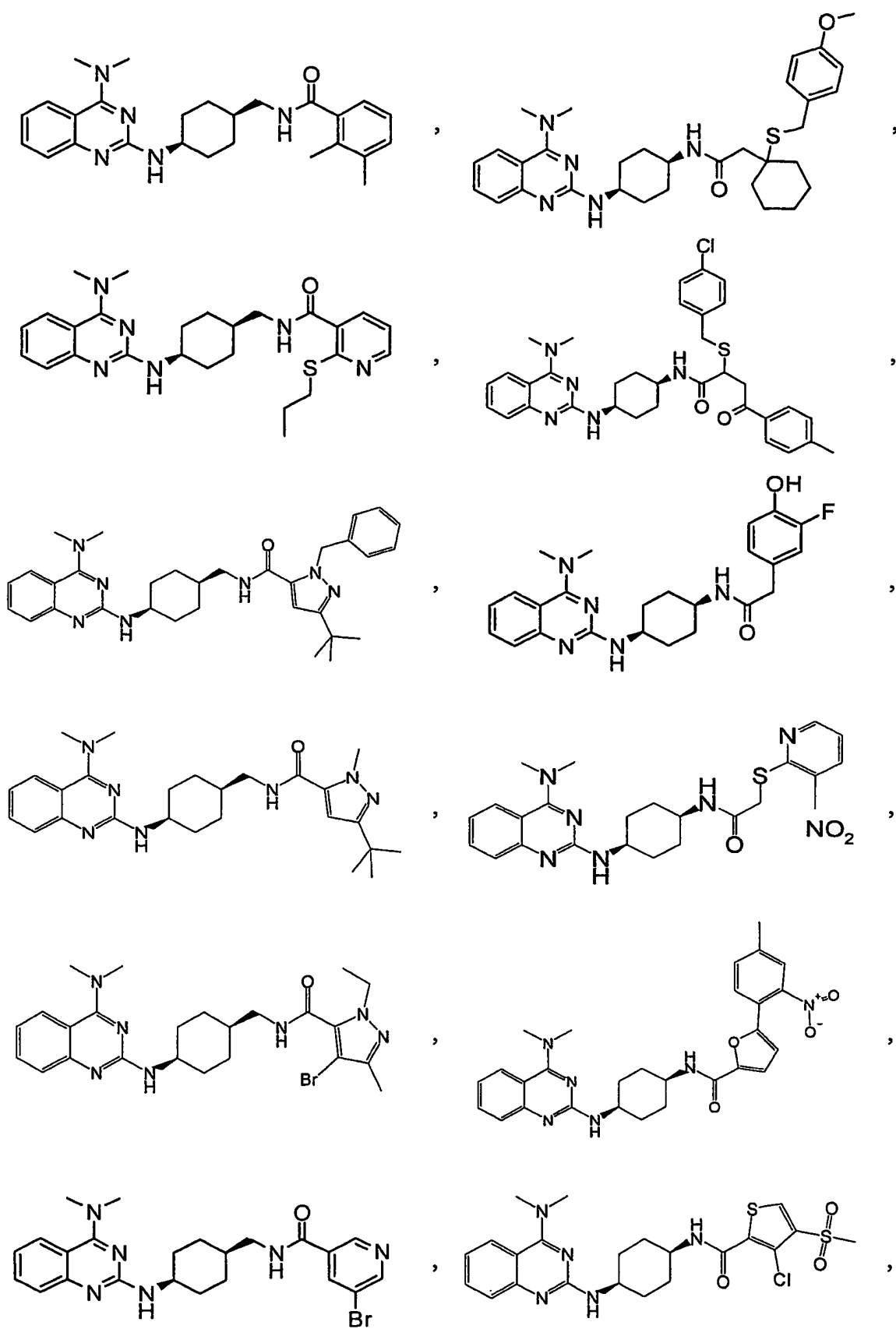


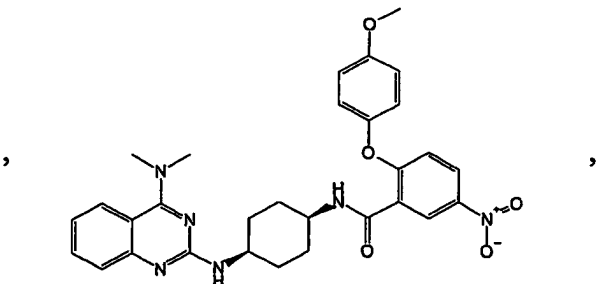
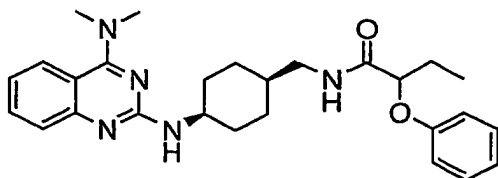
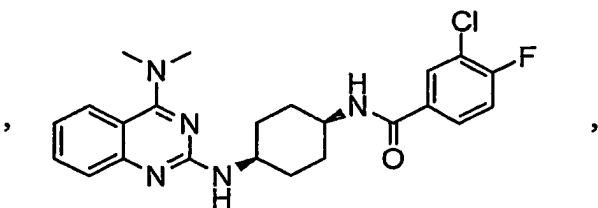
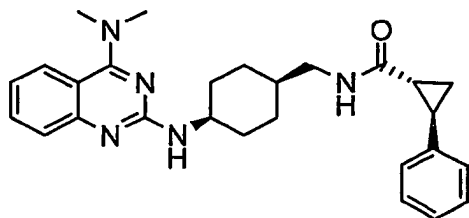
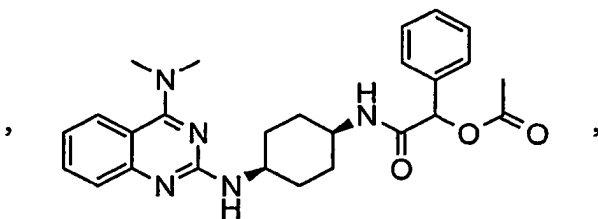
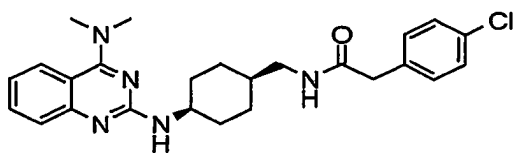
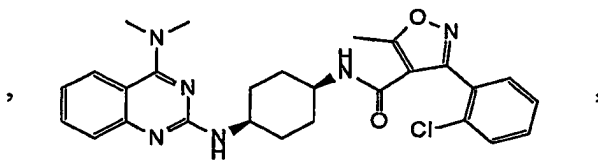
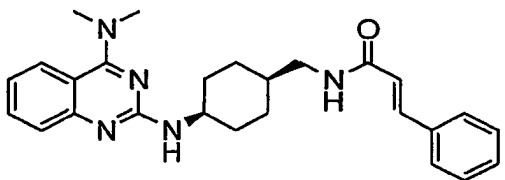
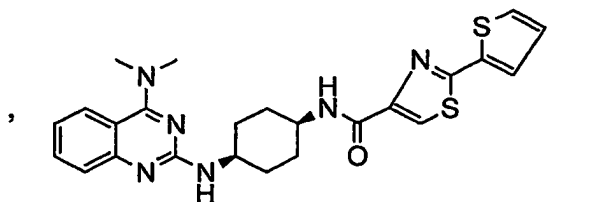
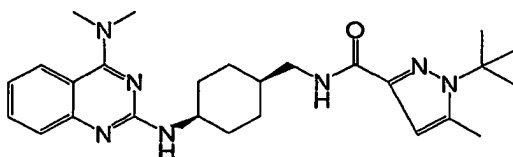
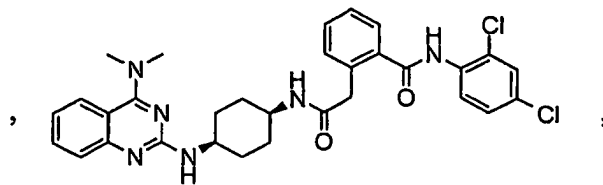
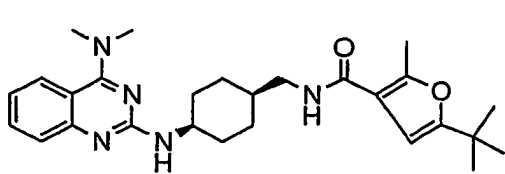


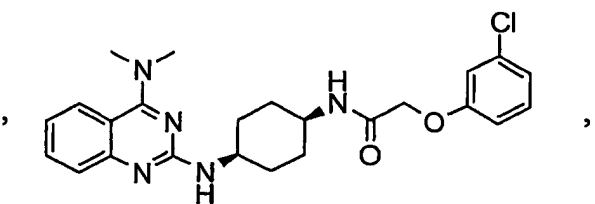
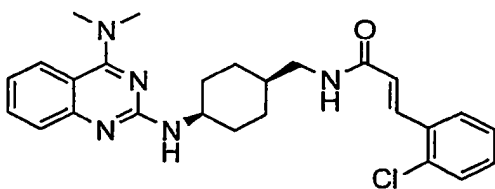
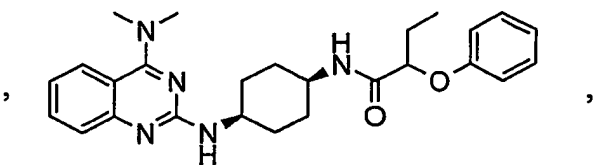
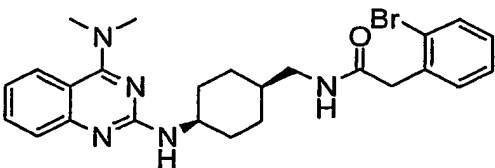
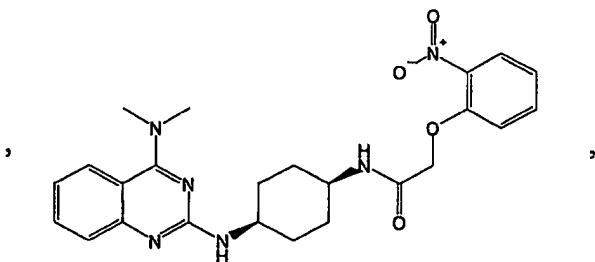
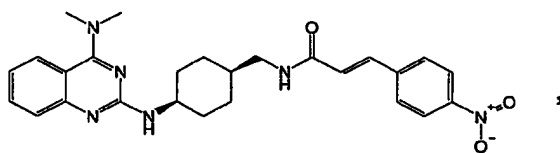
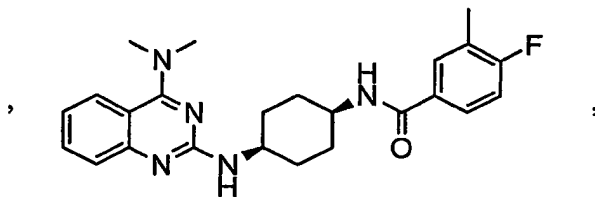
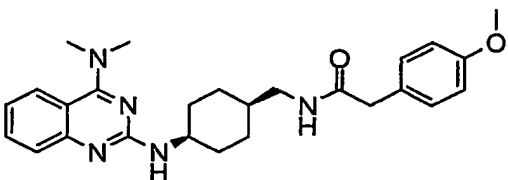
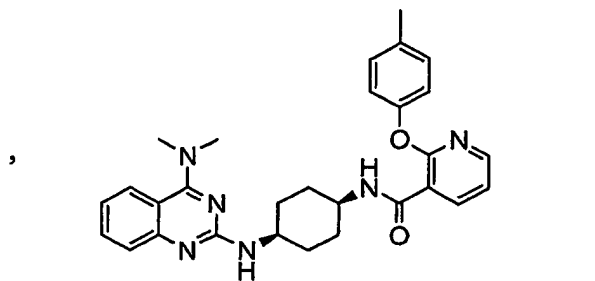
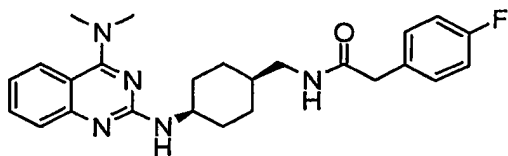
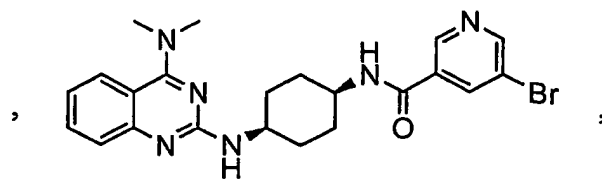
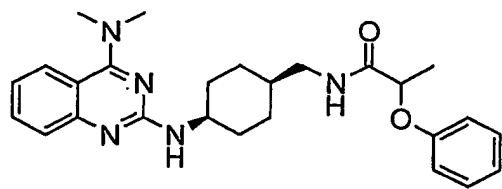


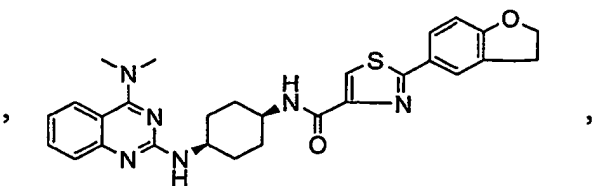
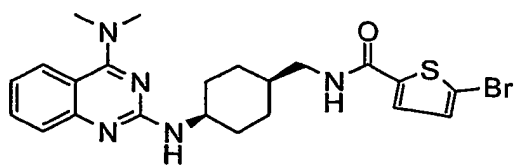
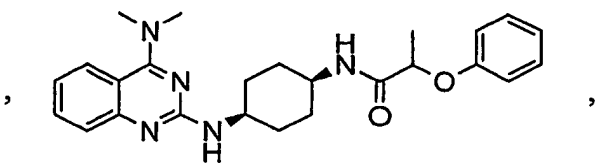
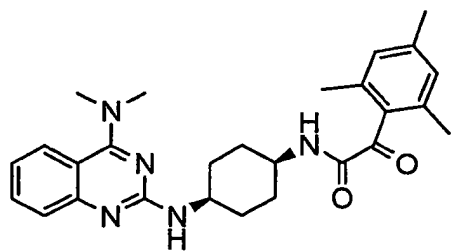
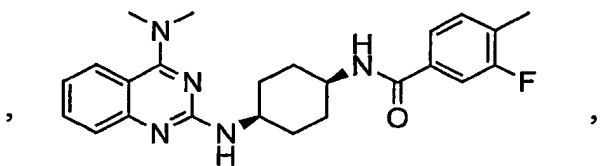
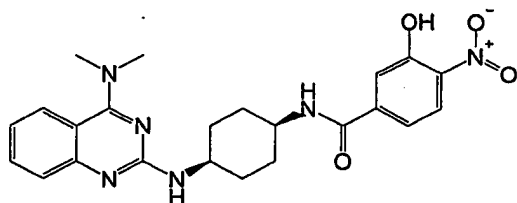
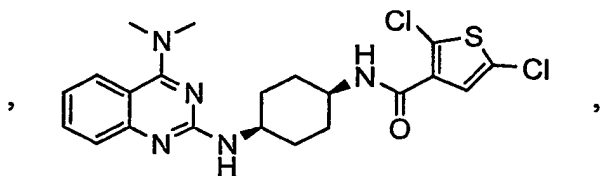
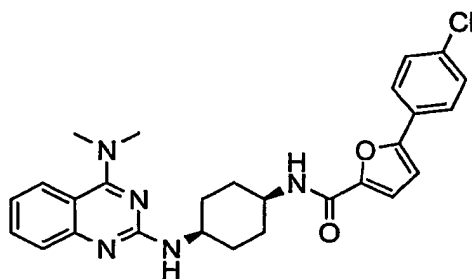
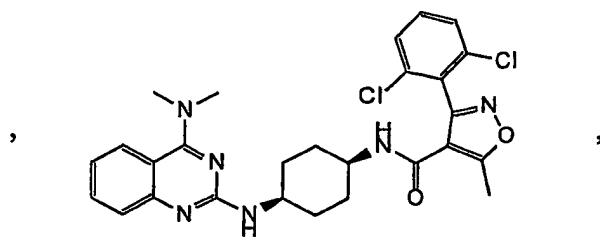
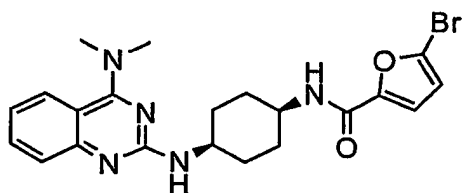
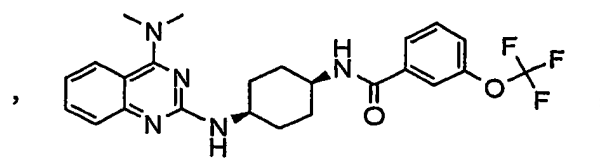
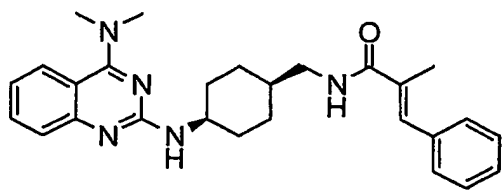


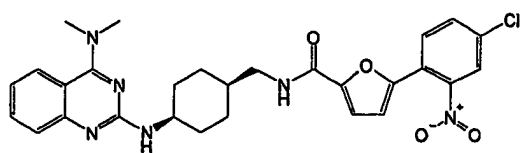




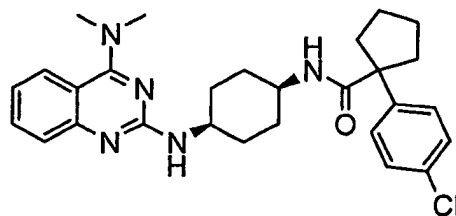




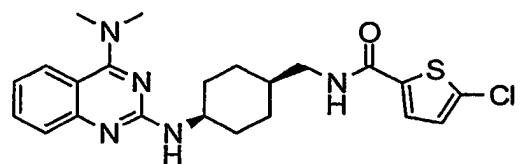




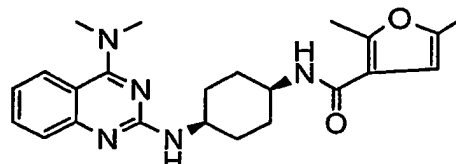
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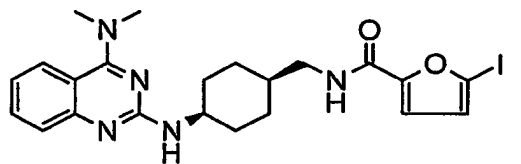
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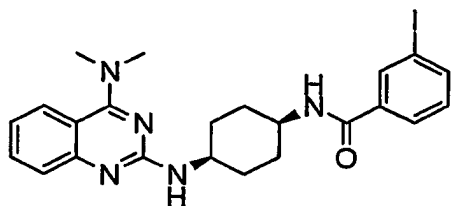
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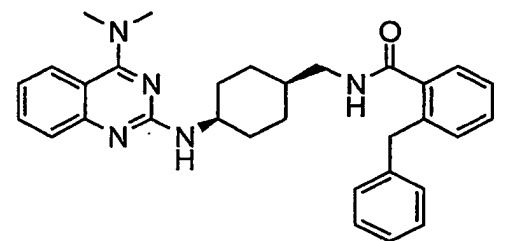
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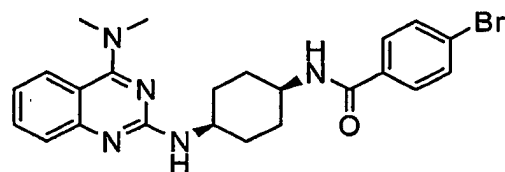
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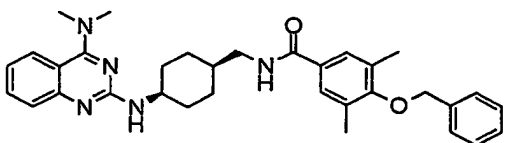
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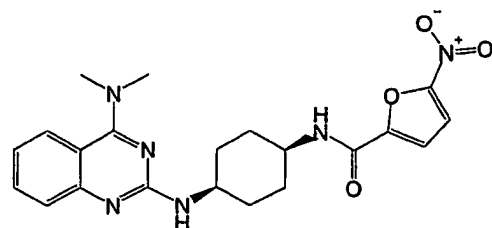
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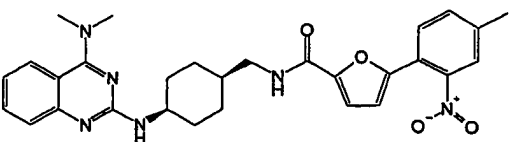
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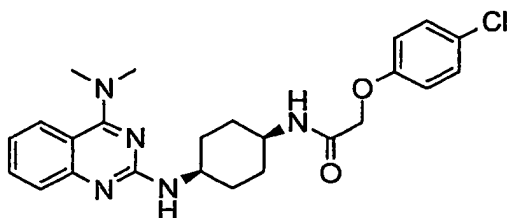
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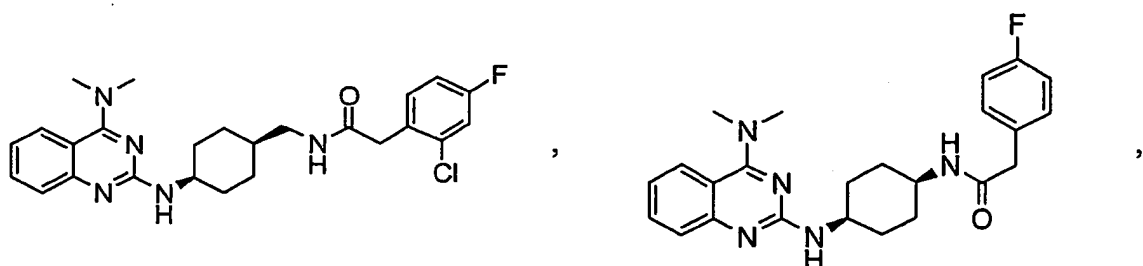
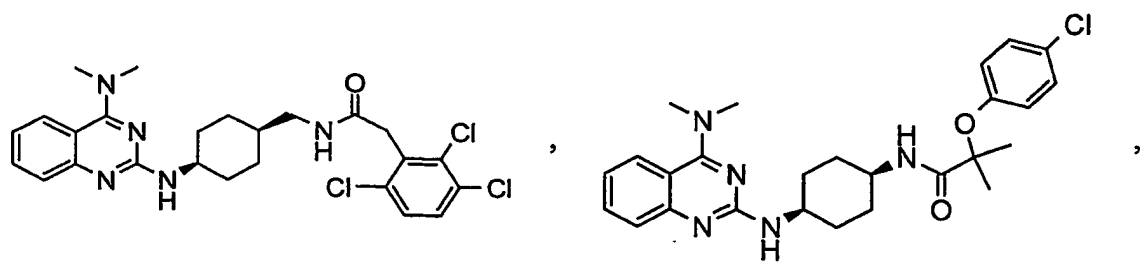
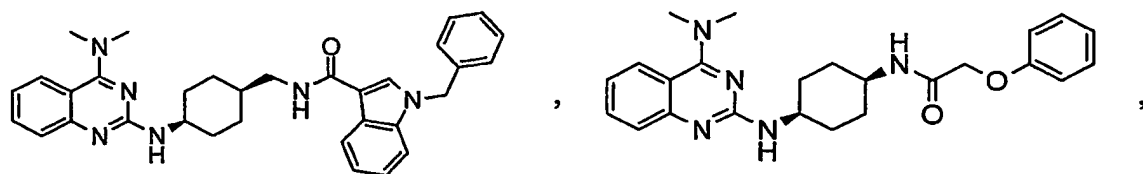
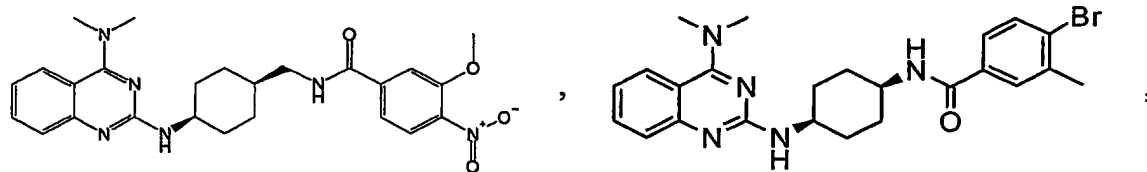
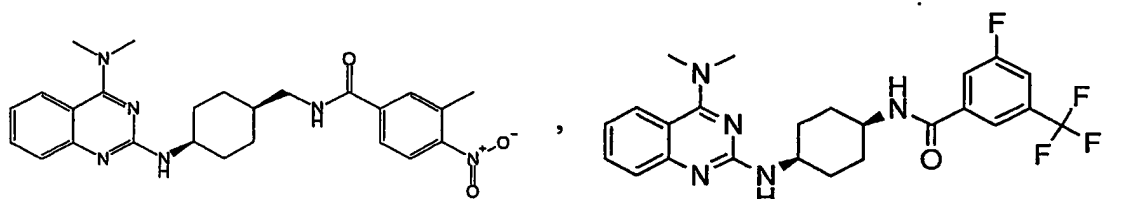
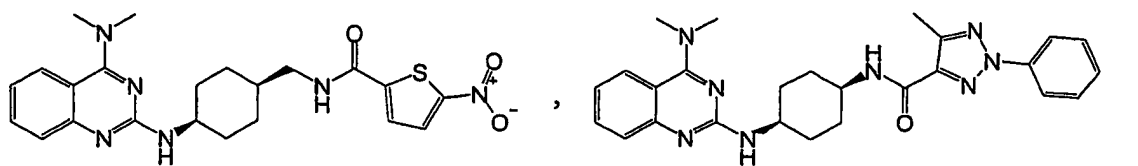
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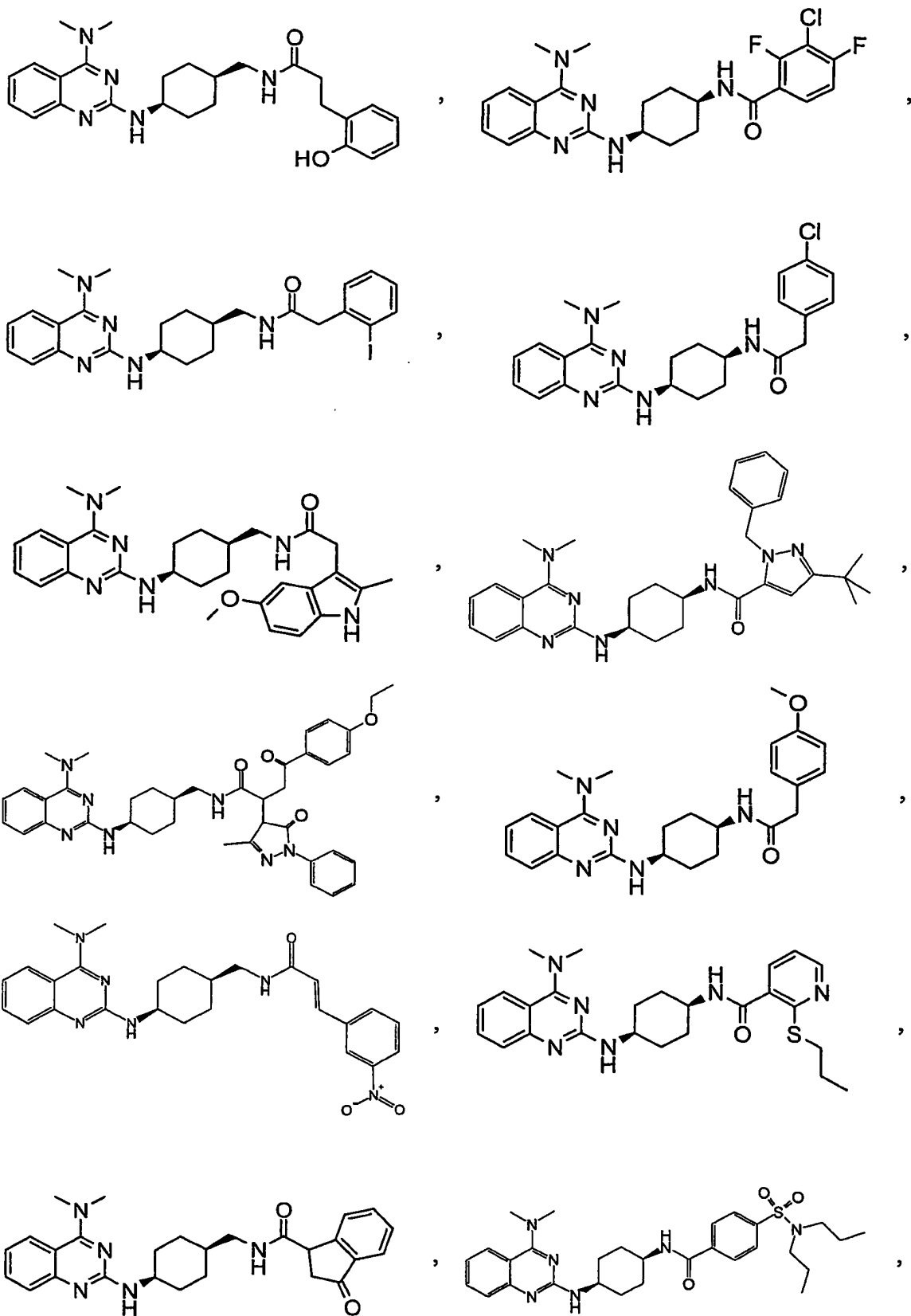


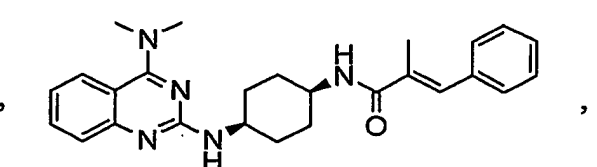
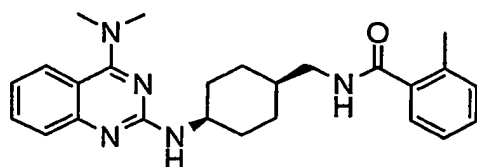
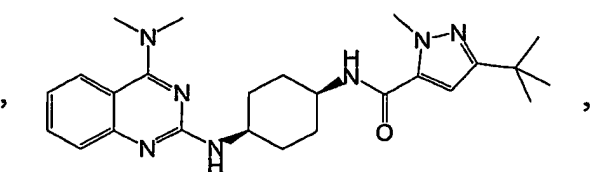
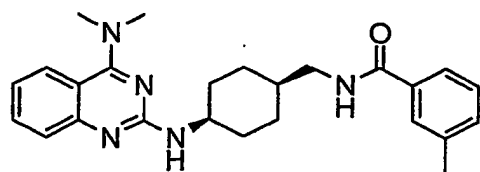
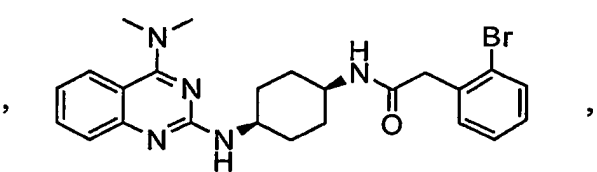
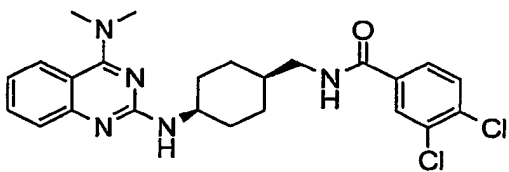
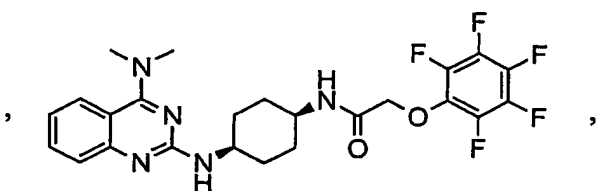
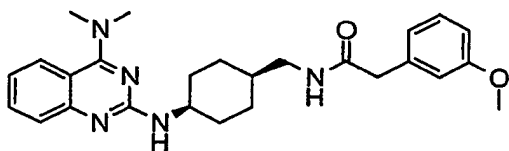
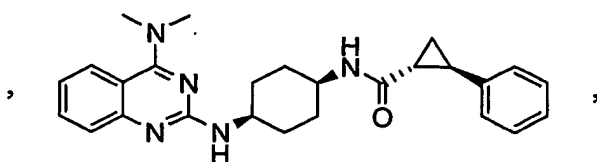
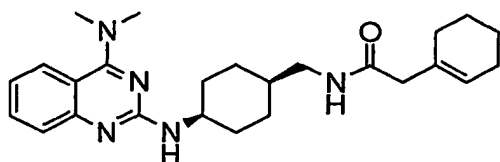
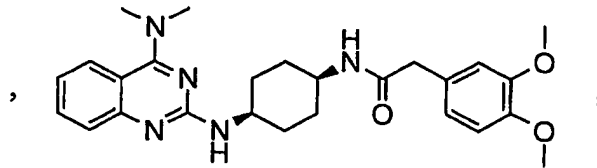
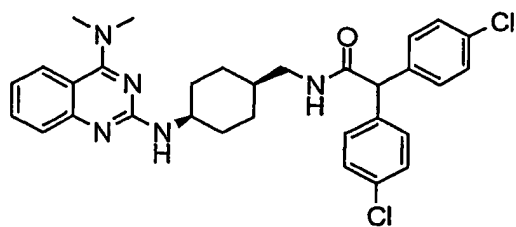
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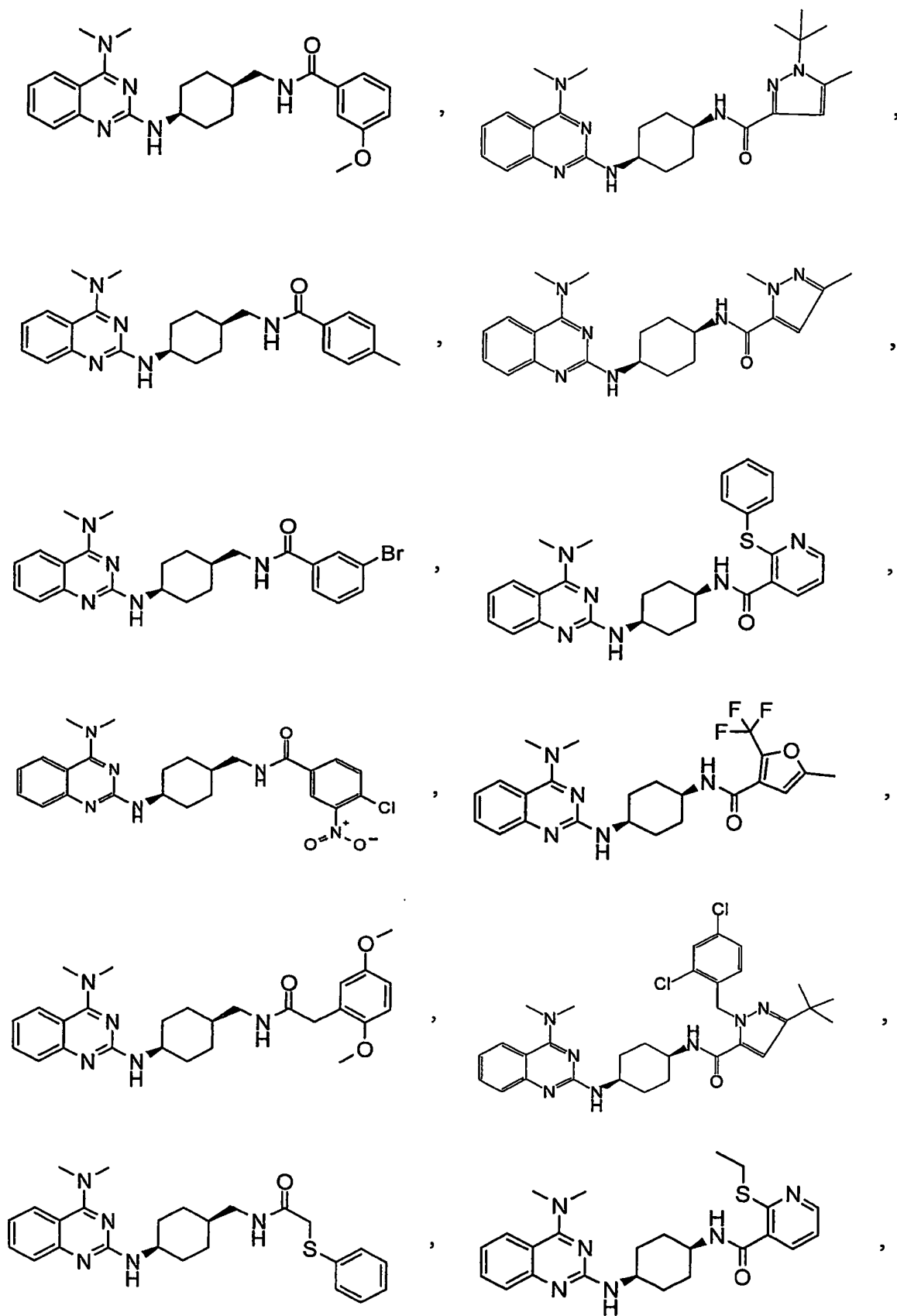


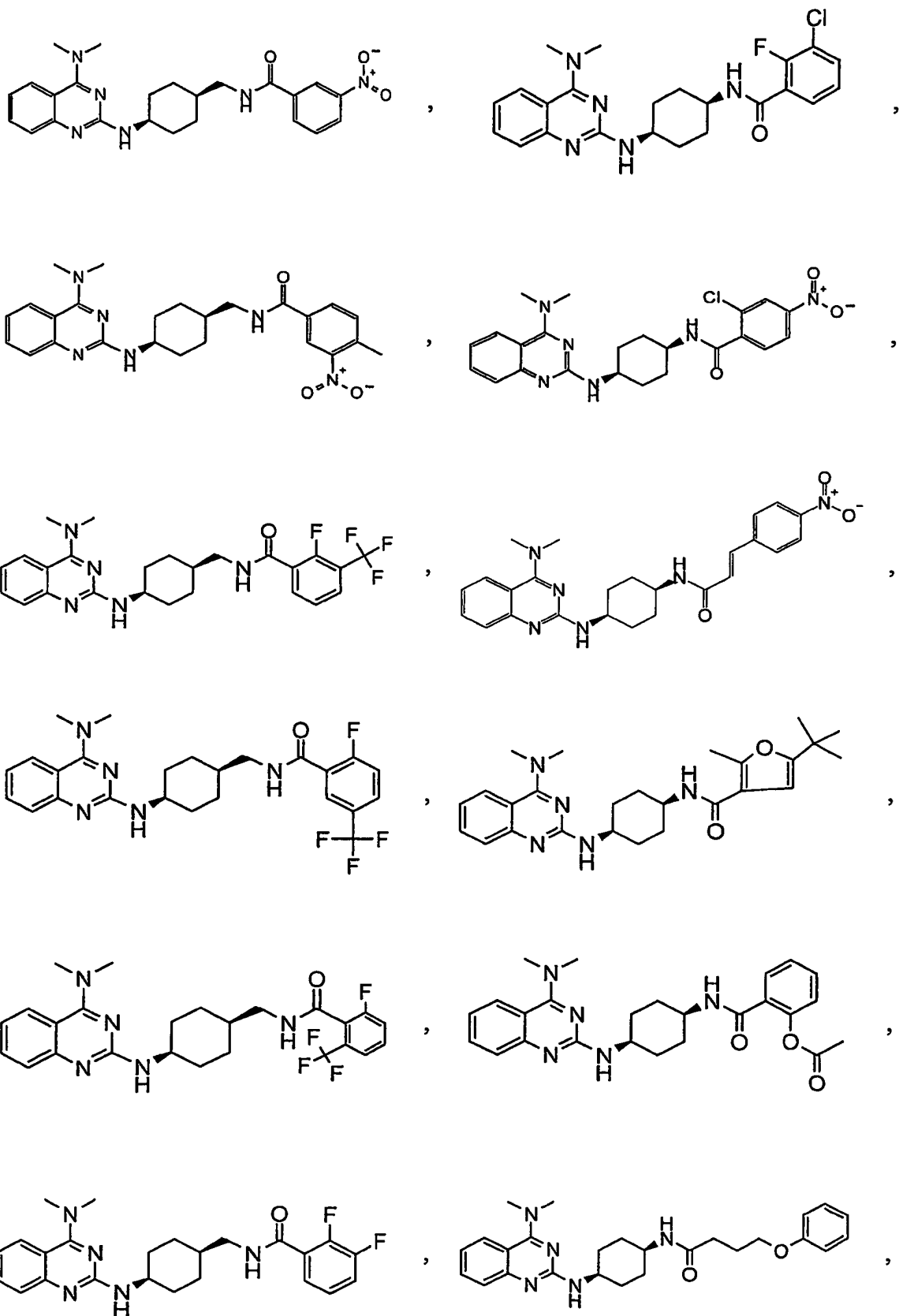
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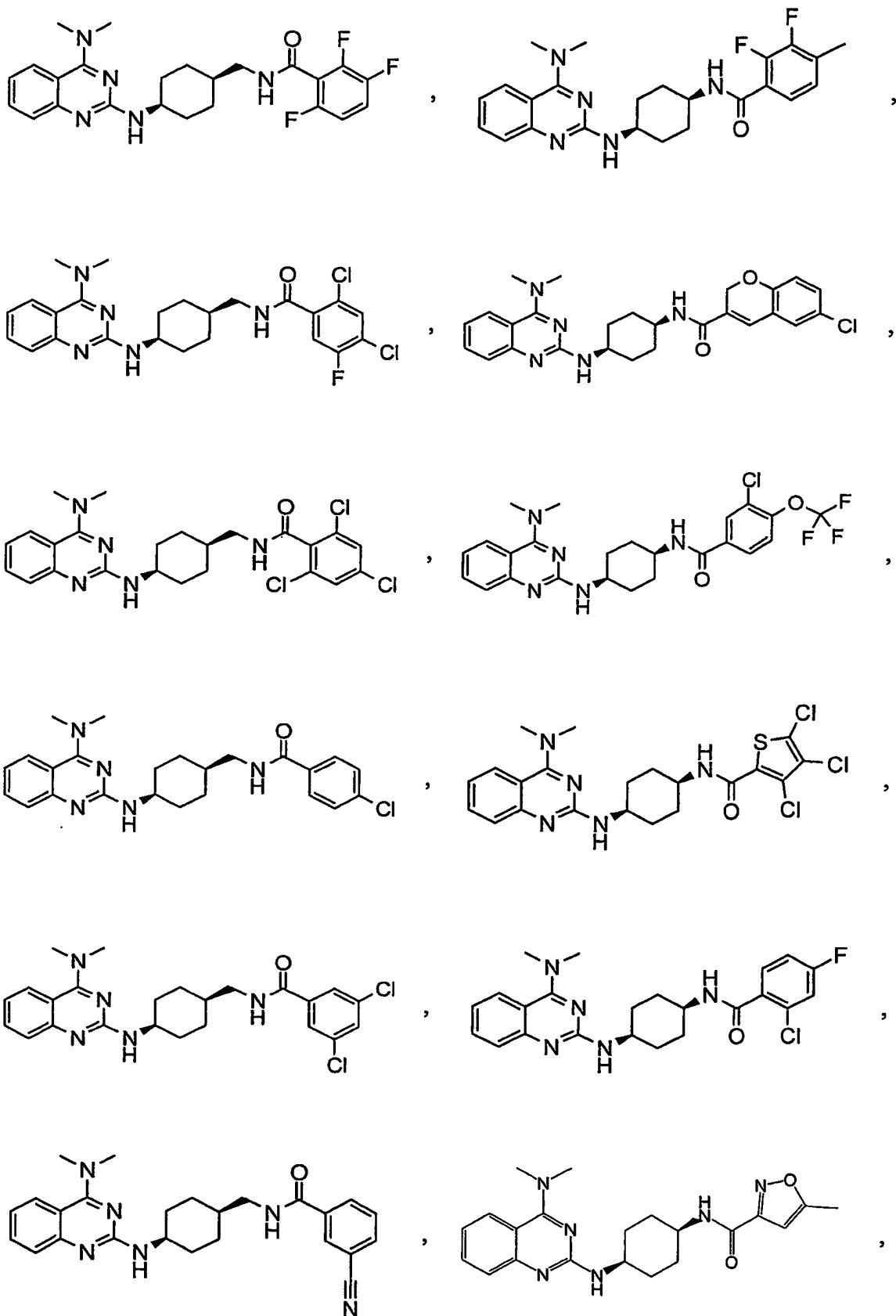


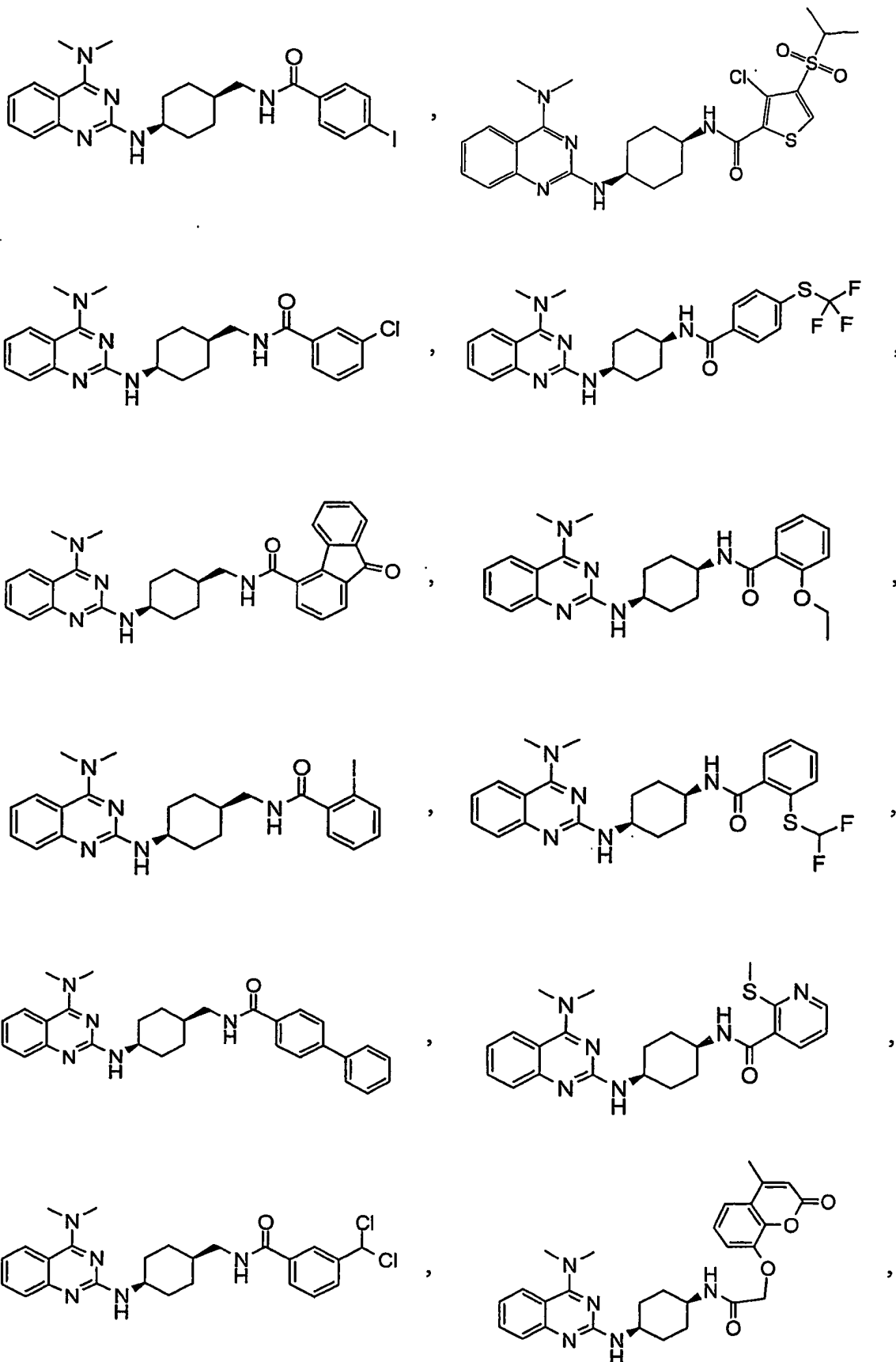


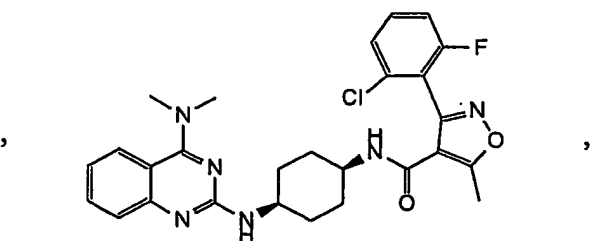
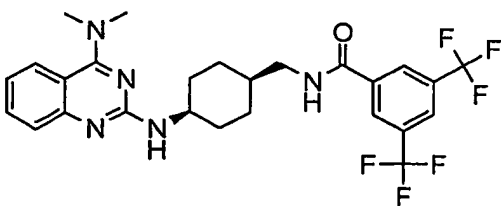
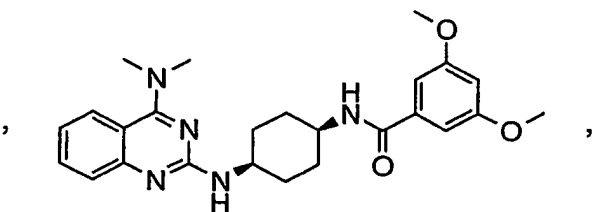
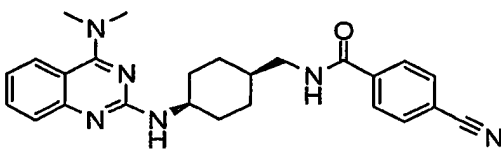
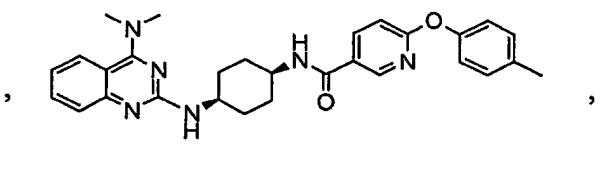
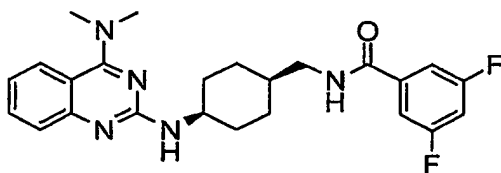
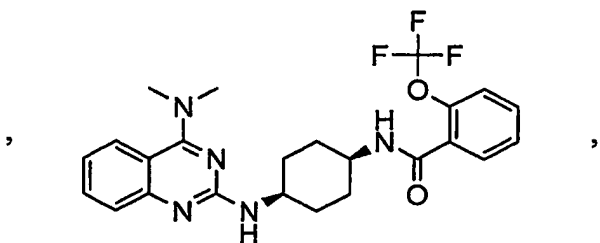
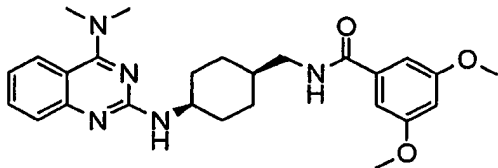
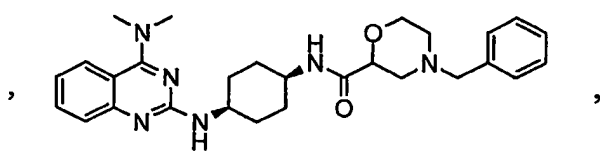
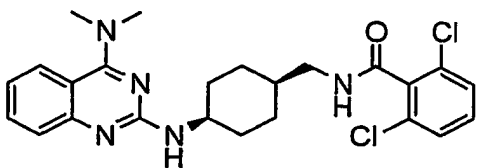
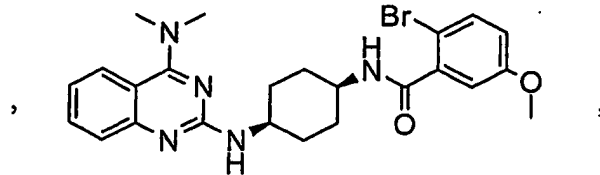
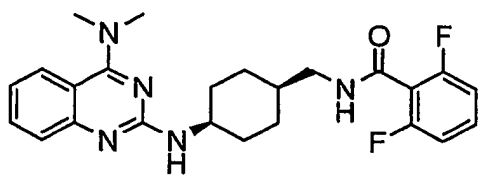


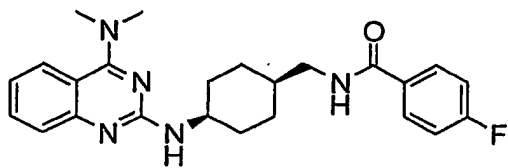




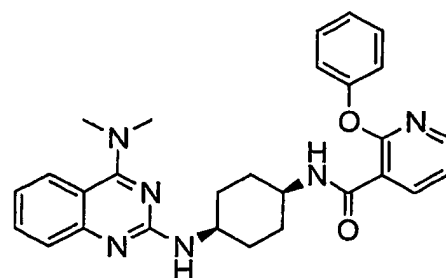




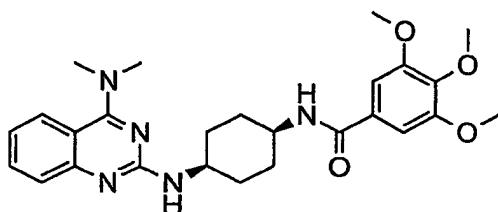




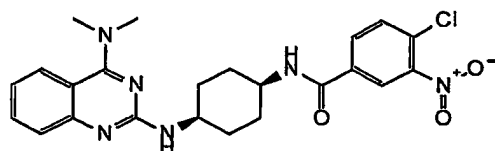
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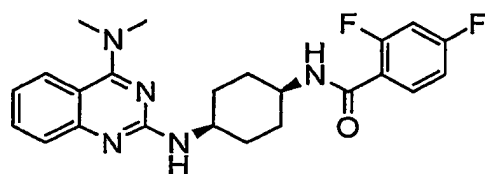
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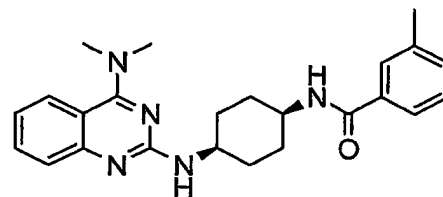
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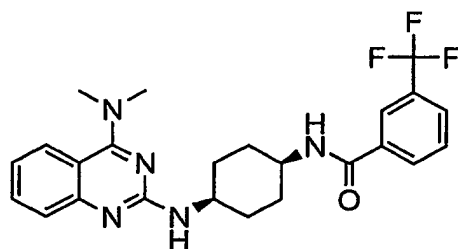
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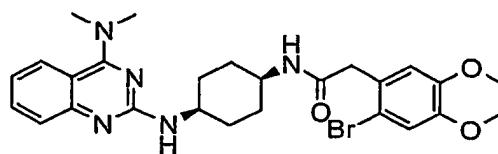
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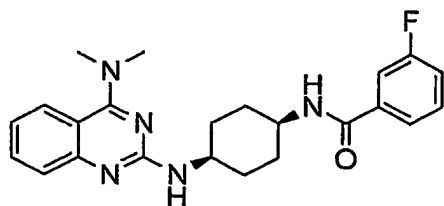
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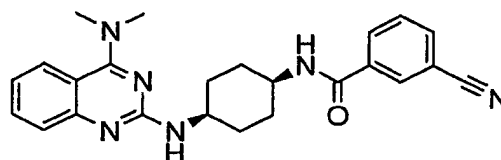
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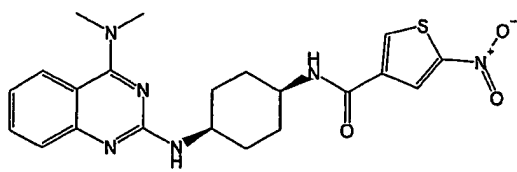
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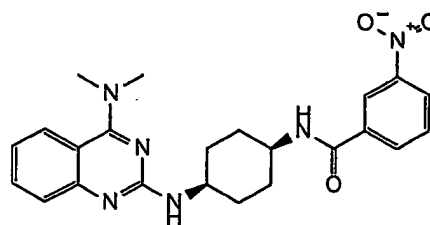
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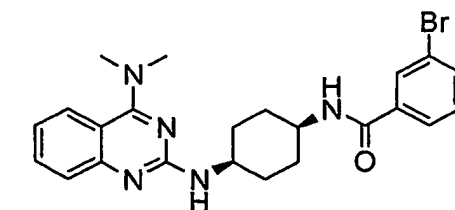
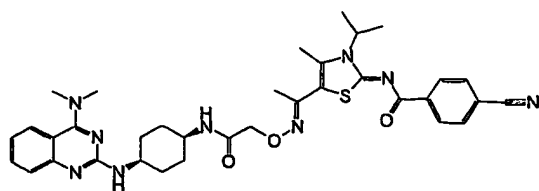
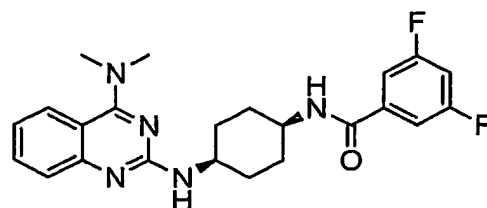
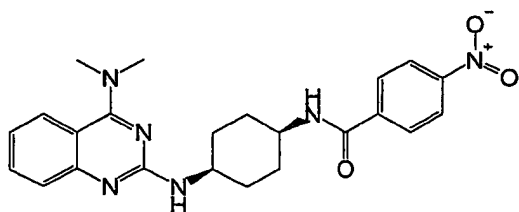
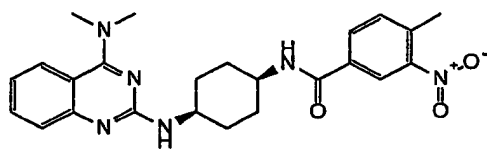
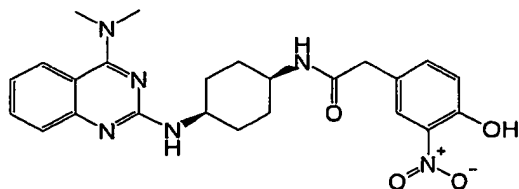
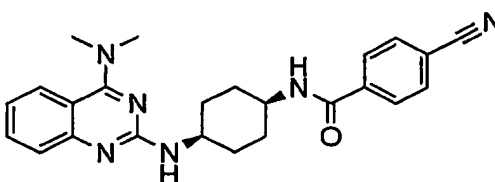
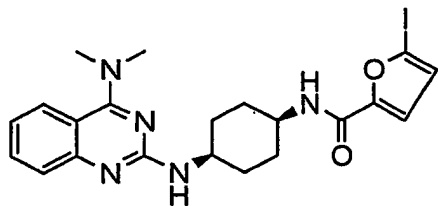
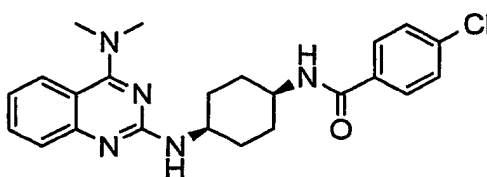
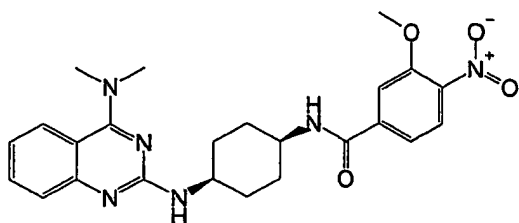
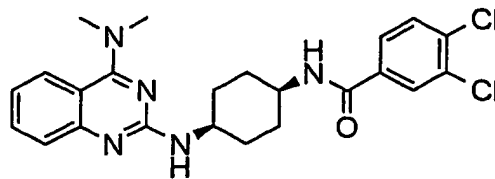
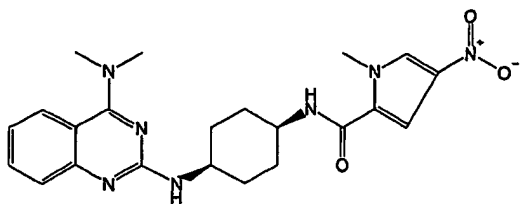
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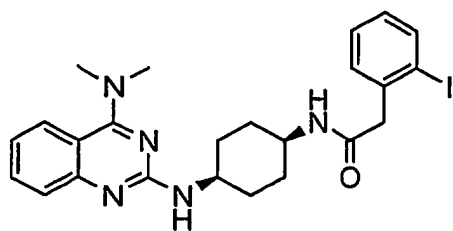


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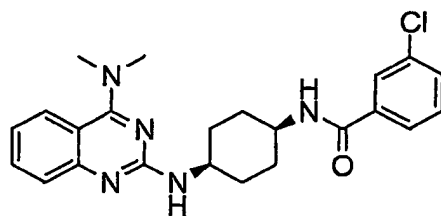


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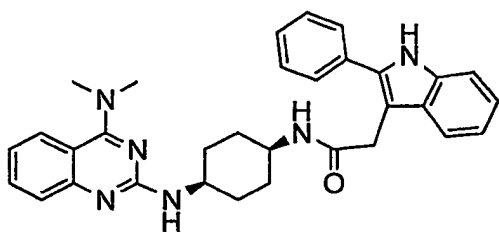




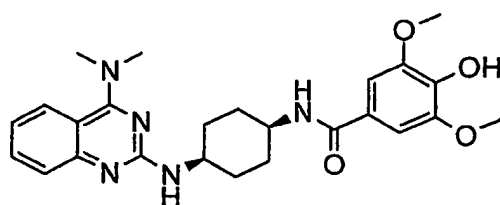
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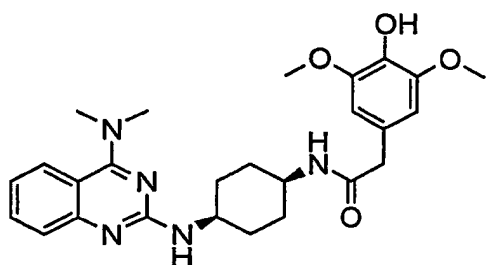
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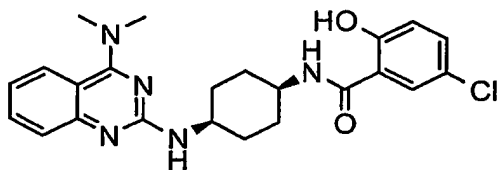
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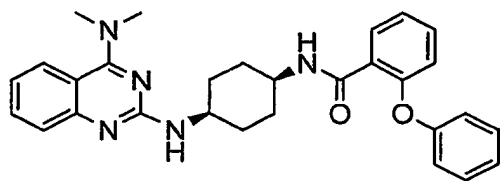
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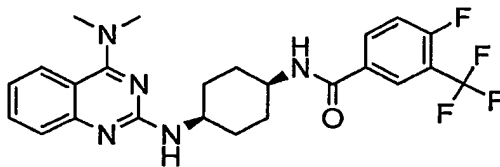
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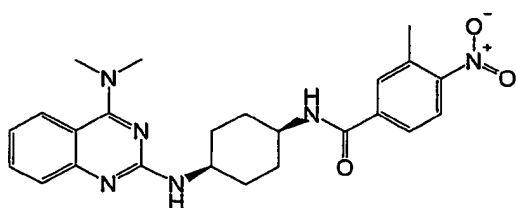
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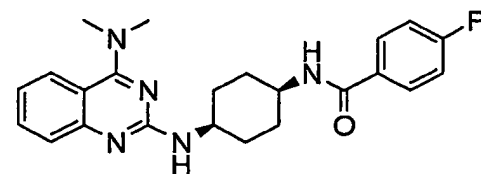
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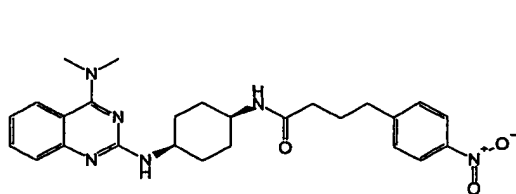
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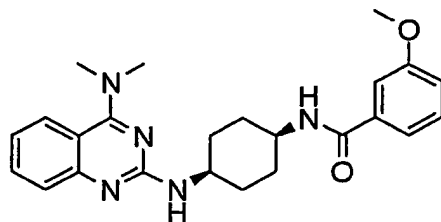
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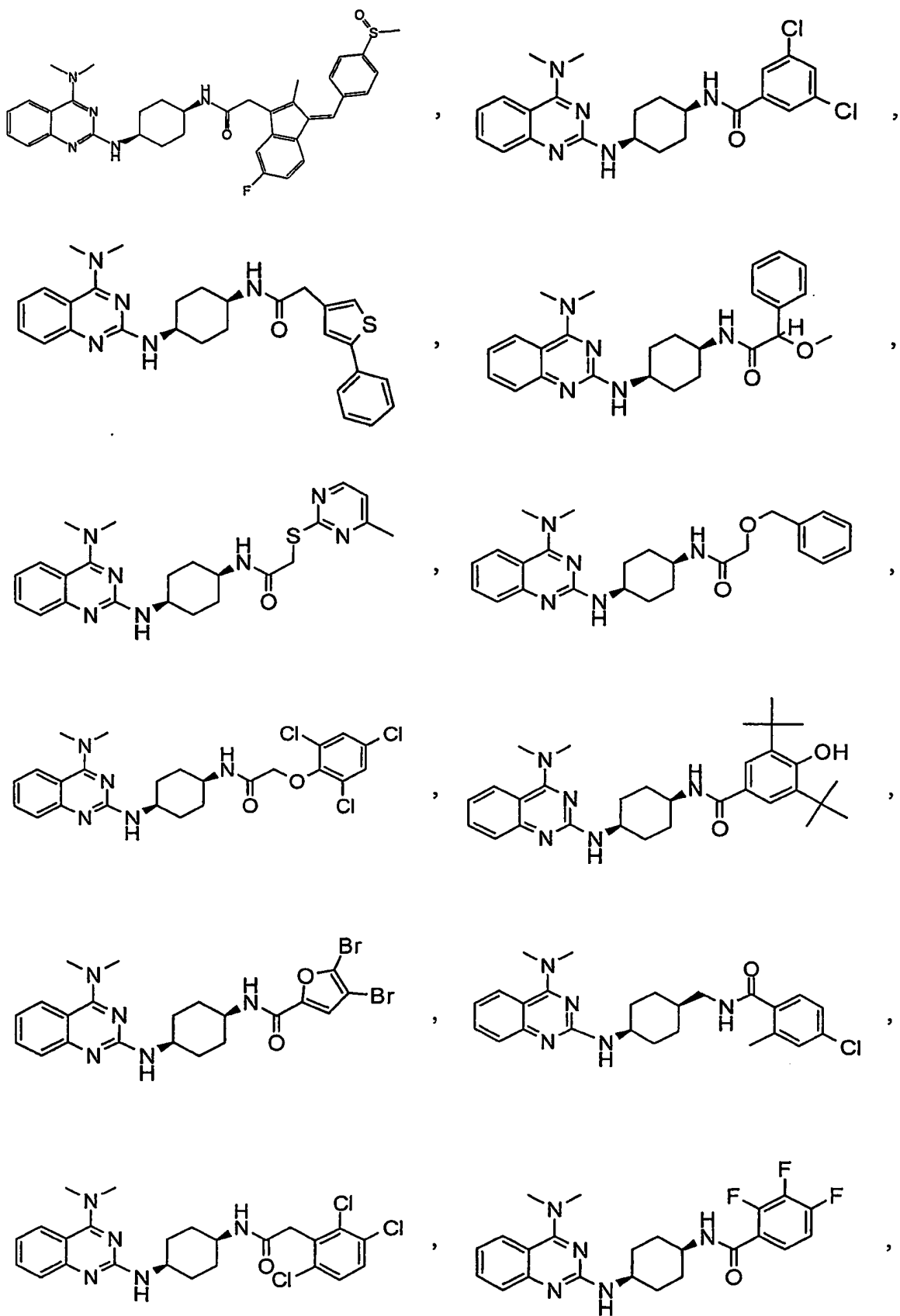
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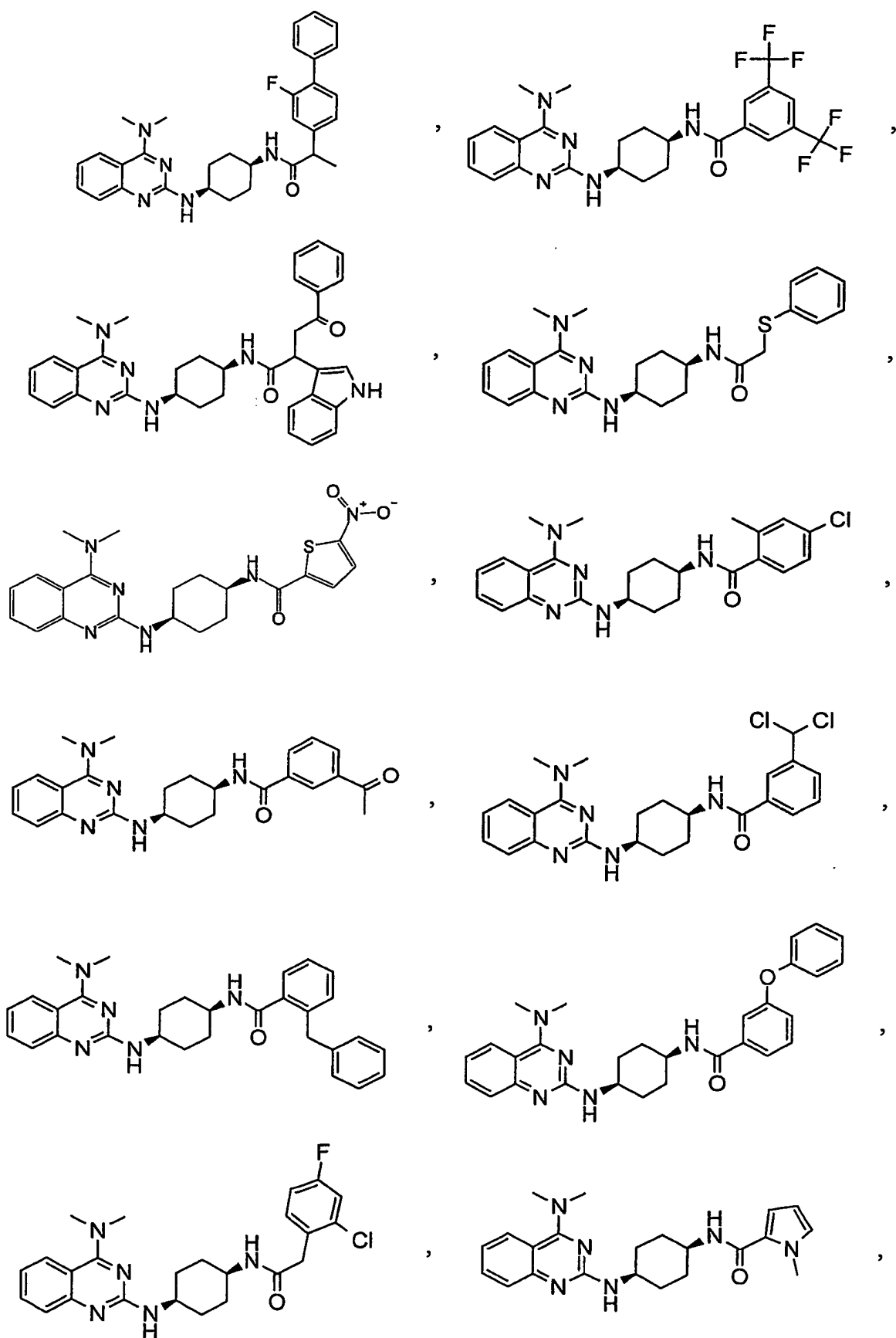


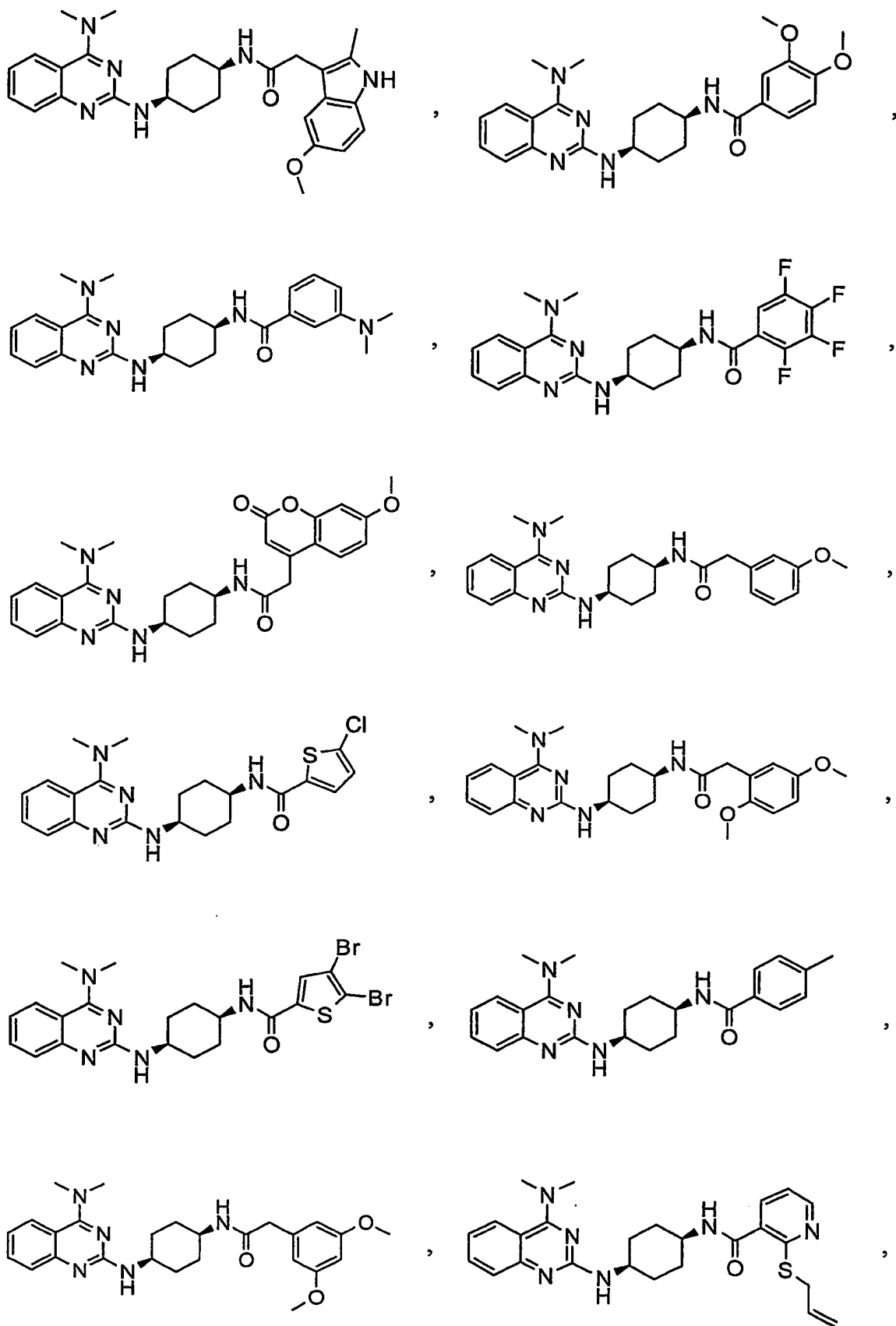
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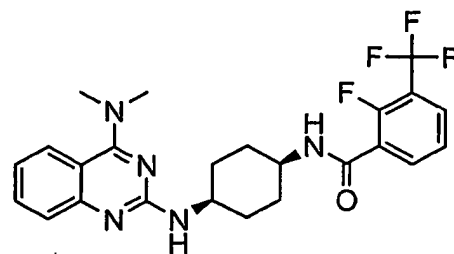
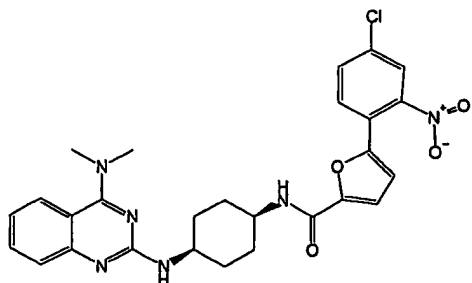
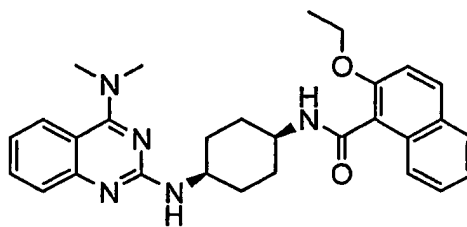
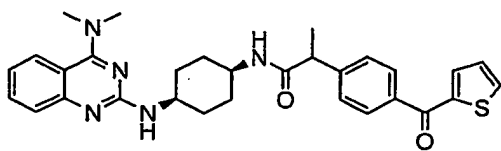
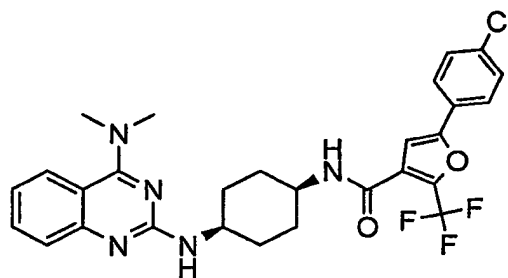
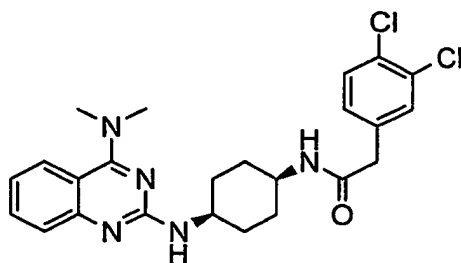
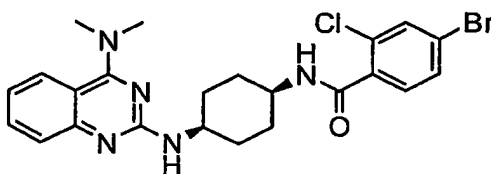
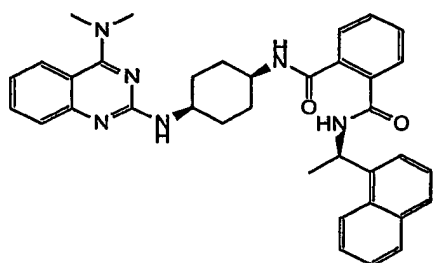
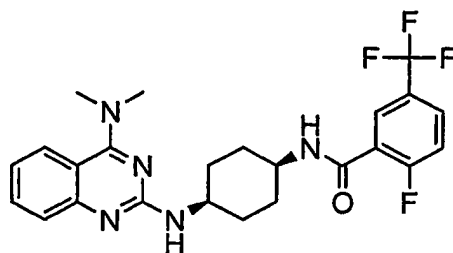
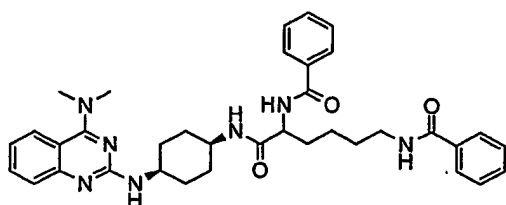
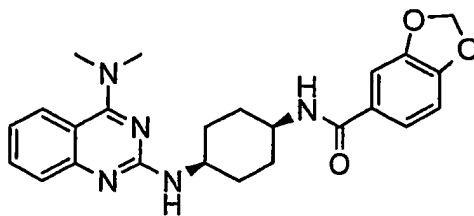
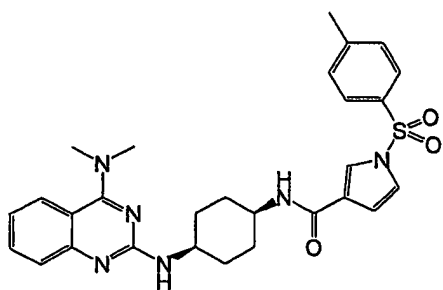


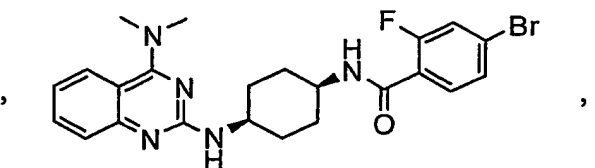
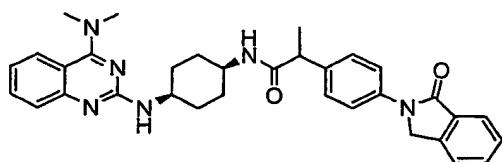
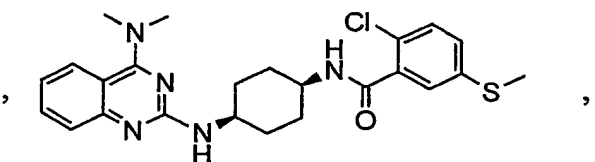
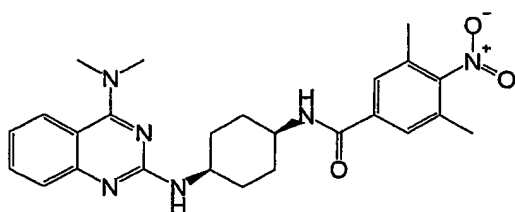
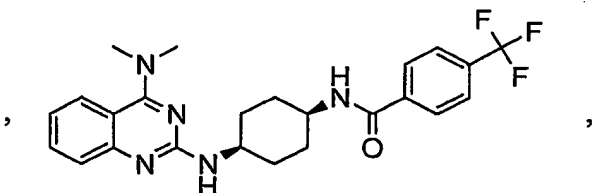
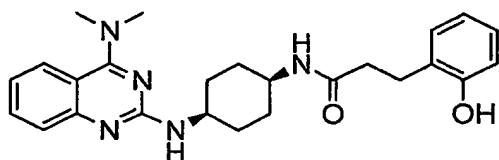
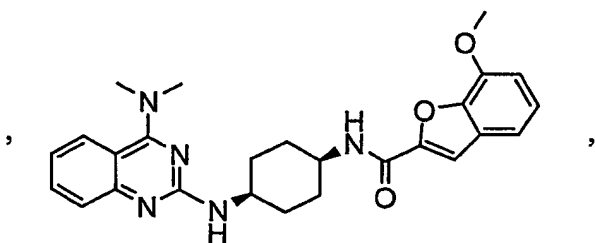
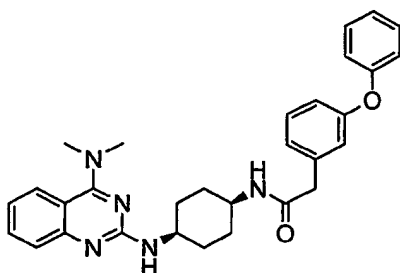
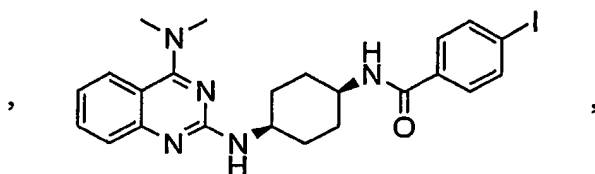
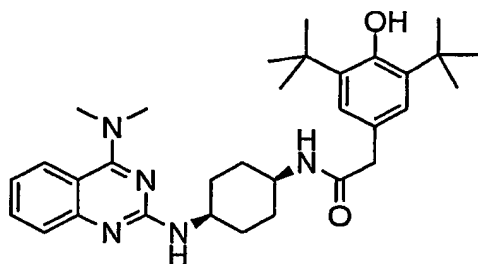
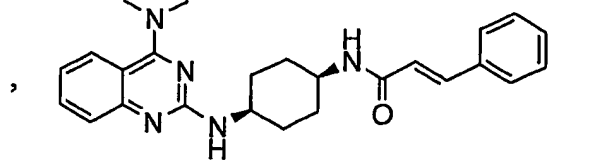
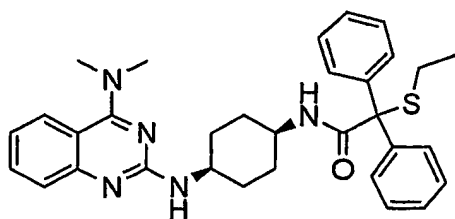
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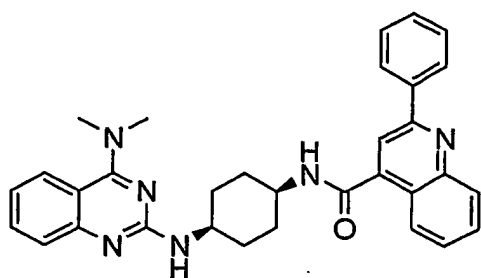




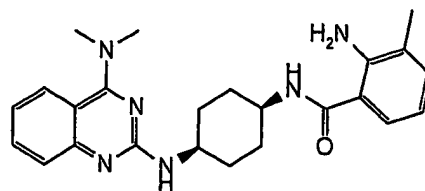




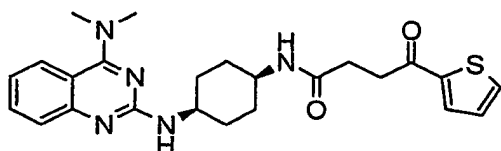




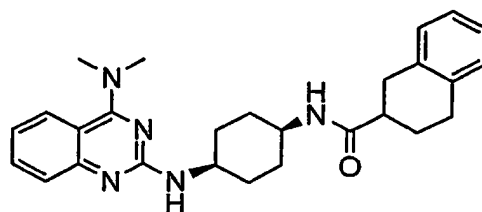
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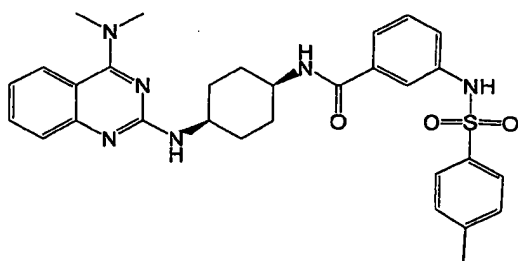
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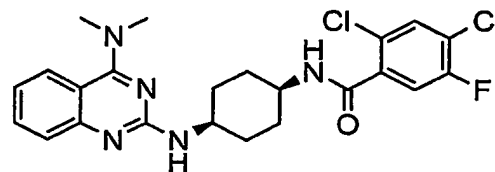
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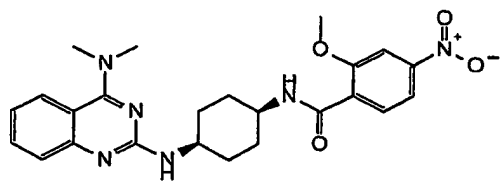
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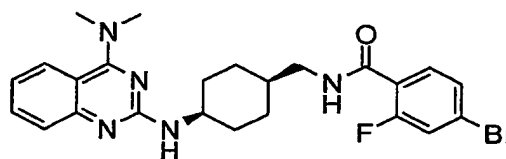
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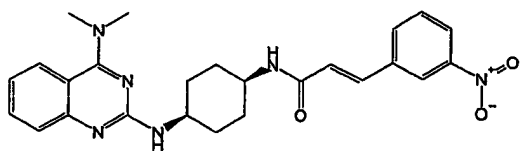
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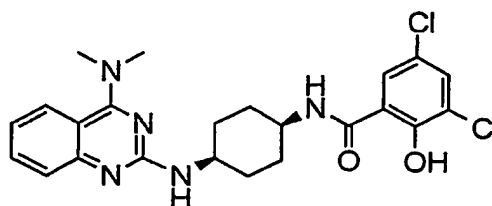
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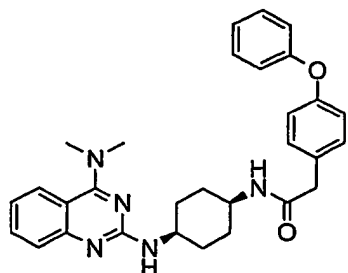
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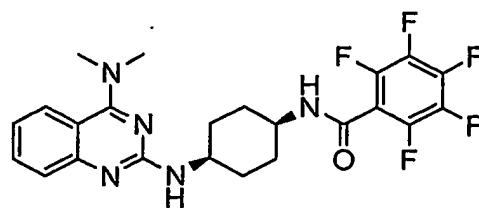
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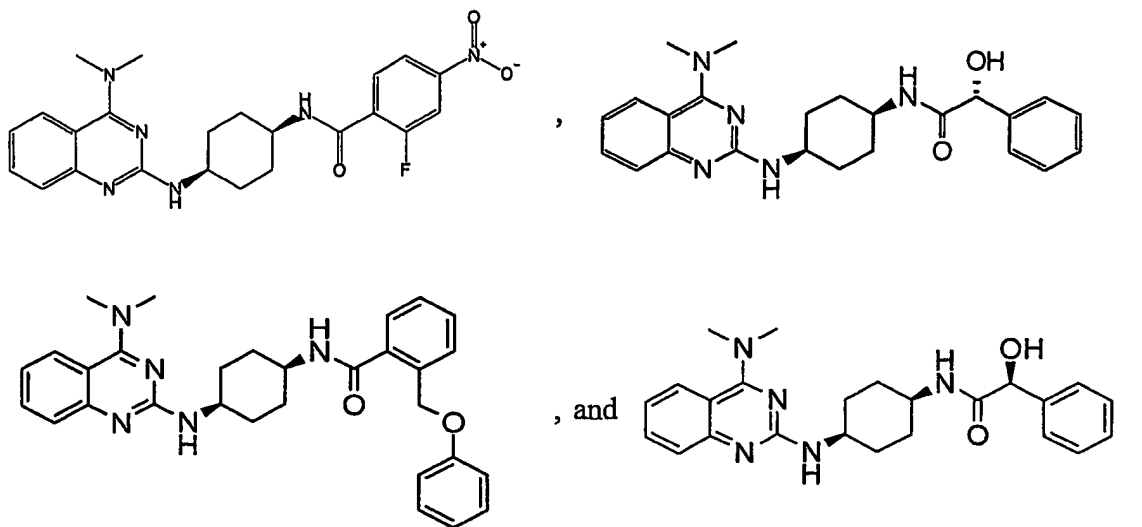
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; or, in case of, a salt thereof.

7. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

•C₅-C₆ cycloalkyl,

•carbocyclic aryl,

•heterocyclyl,

(ii) C₃-C₆ cycloalkyl,

(iii) carbocyclic aryl,

(iv) or heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 1,3-dioxo-isoindolyl, 1*H*-indolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, oxolanyl, piperidyl, pyridyl, quinoxalyl, thienyl, quinolyl, or benzothiazolyl; or a salt thereof.

8. A compound according to claim 7, wherein

R₁ represents

(i) C₁-C₄ alkyl,

C₁-C₄ alkyl substituted by substituent(s) independently selected from

•cyclopentyl,

•carbocyclic aryl,

•heterocyclyl,

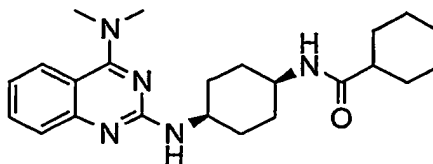
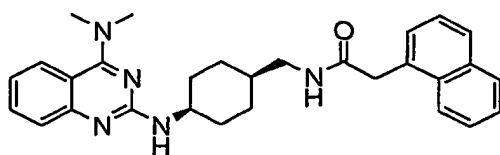
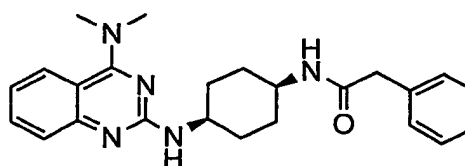
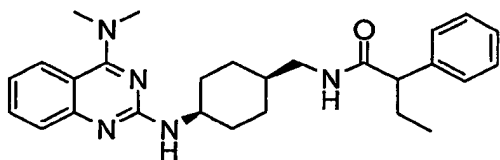
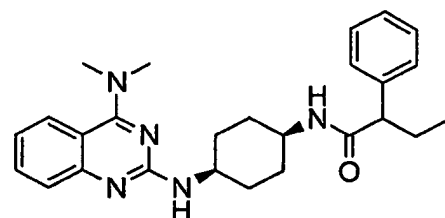
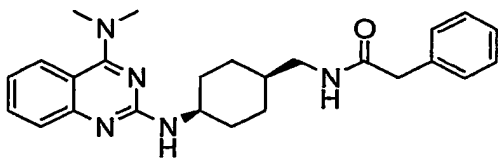
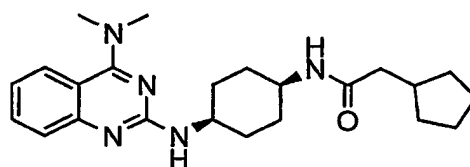
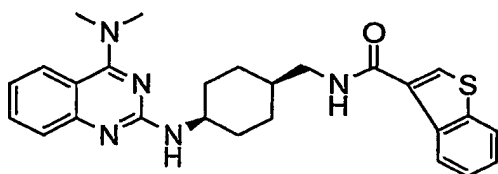
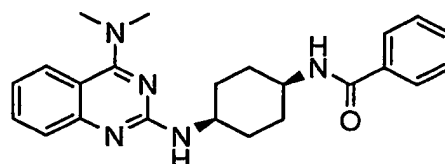
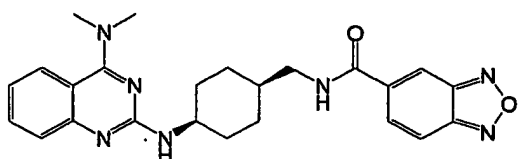
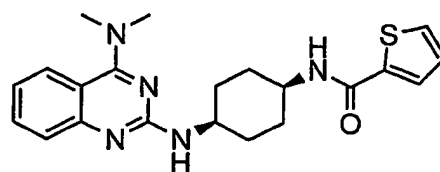
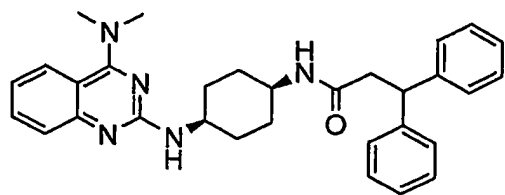
(ii) carbocyclic aryl,

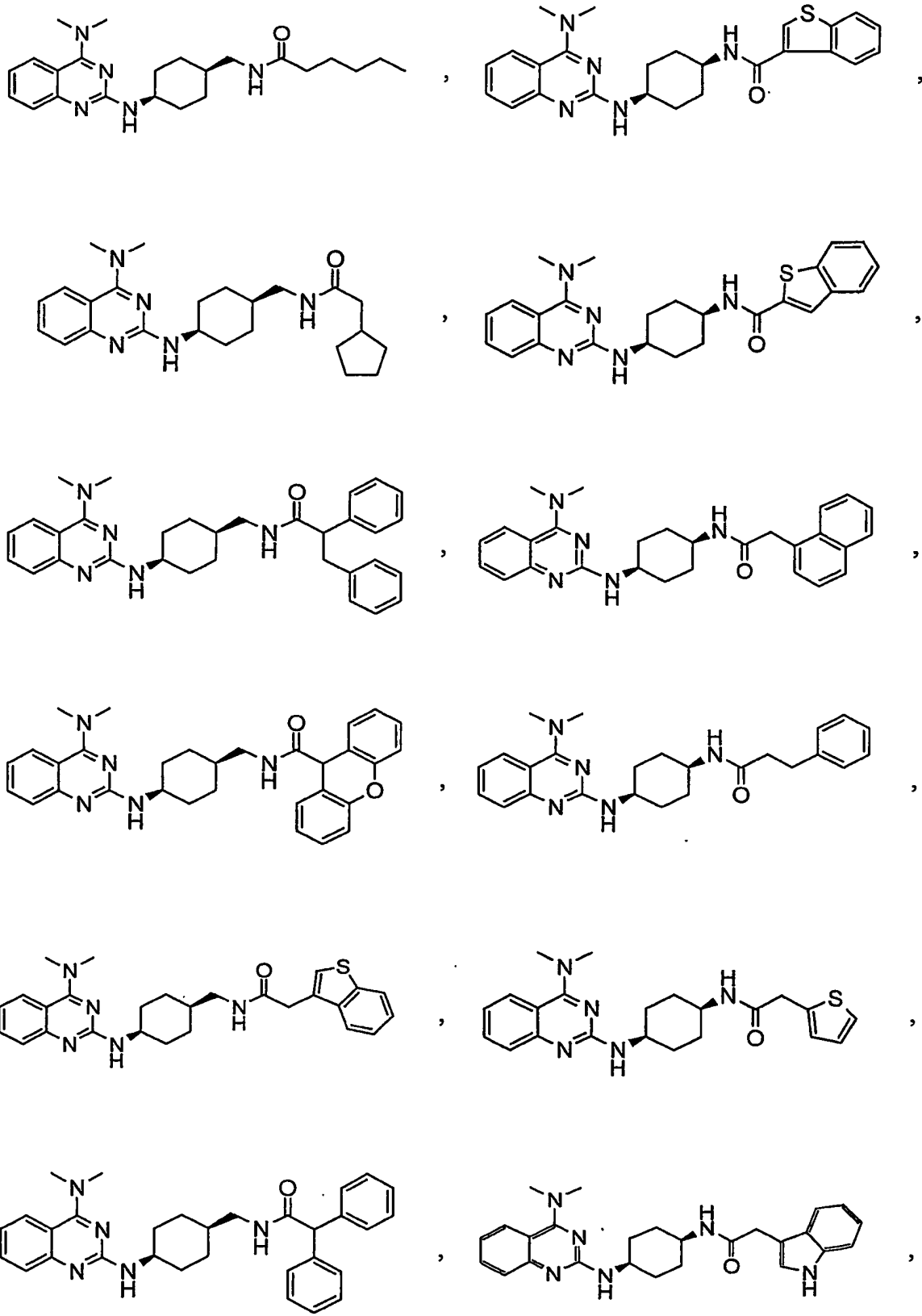
(iii) or heterocyclyl;

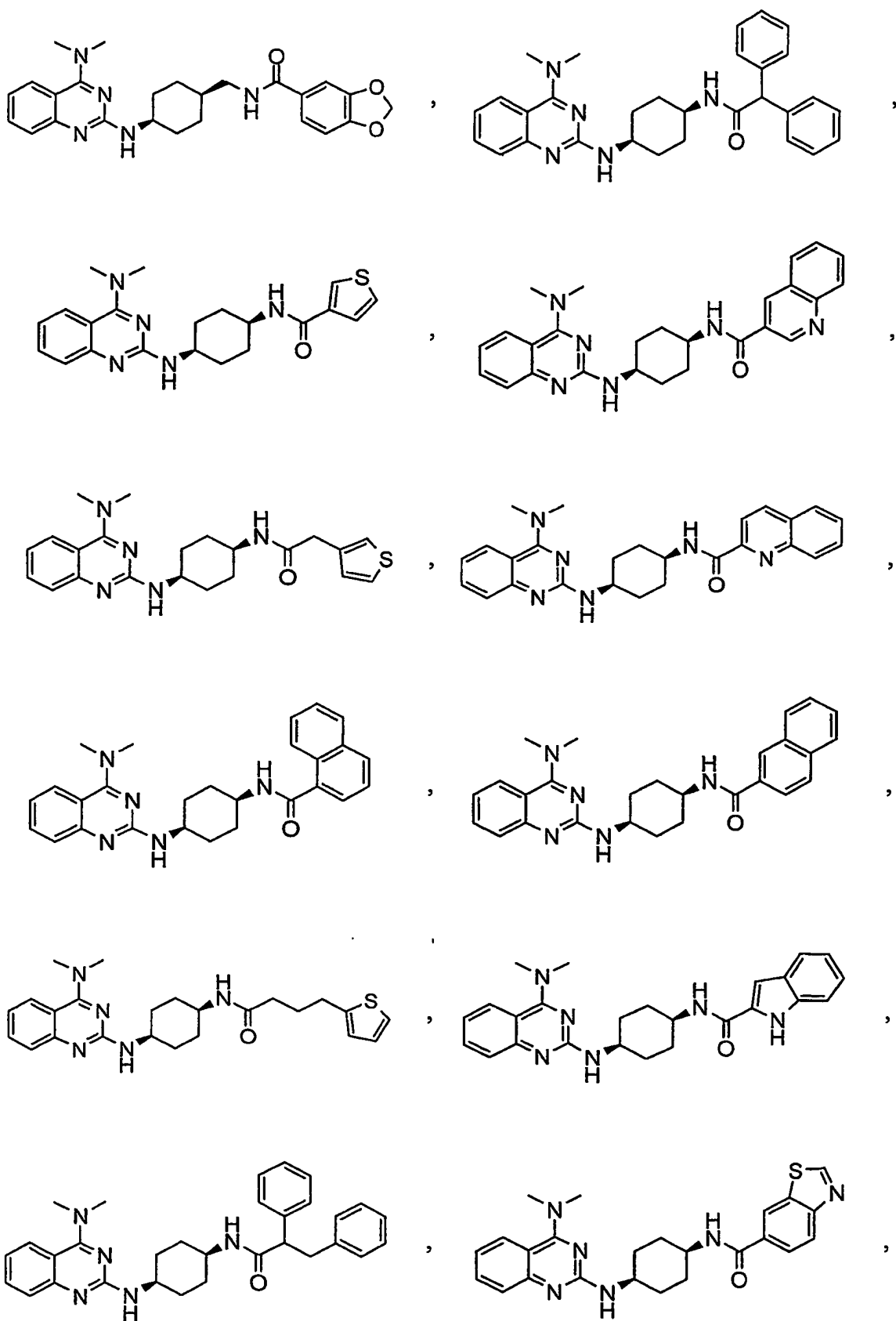
wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

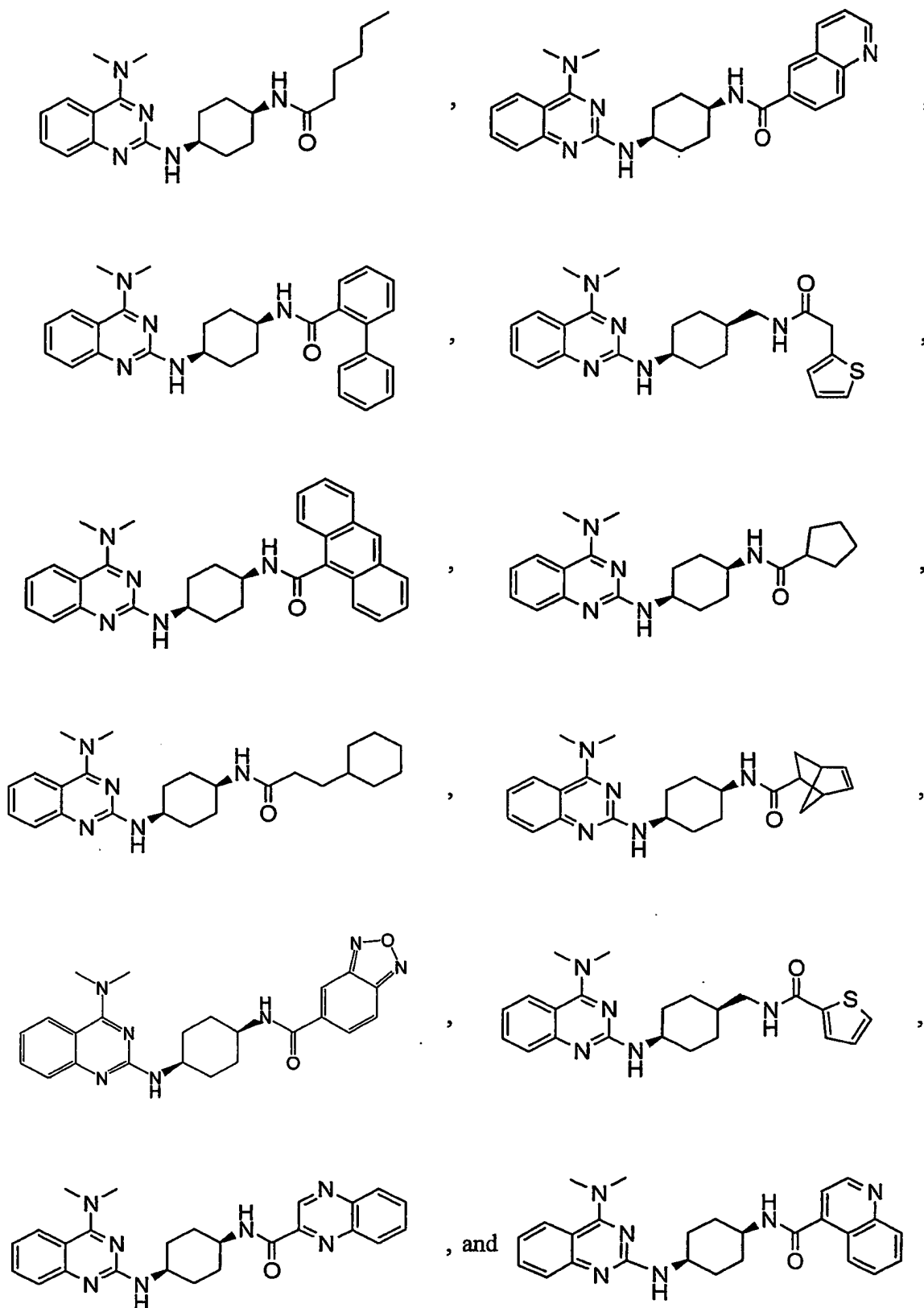
heterocyclyl is 9*H*-xanthenyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, thienyl, 1*H*-indolyl, quinoxalyl, quinolyl, or benzothiazolyl; or a salt thereof.

9. A compound according to claim 8 of Formula I thereof selected from the group consisting of









; or, in case of, a salt thereof.

10. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

- (i) C₁-C₁₀ alkyl,
- C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by C₁-C₃ alkoxy,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
 - cyano,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylcarbonylamino,
 - C₁-C₄ alkoxycarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
- carbocyclic arylsulfonyl,
- halogenated carbocyclic arylsulfonyl,
- heterocyclylthio,
- C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,

- hydroxy,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
- C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by nitro,
- (iii) C₂-C₄ alkynyl,
- C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (v) C₃-C₆ cycloalkenyl,
- C₃-C₆ cycloalkenyl substituted by C₁-C₃ alkyl,
- (vi) carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from

- hydroxy,
- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₁-C₉ alkoxy,
 - C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- halogen,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₂-C₃ alkenyloxy,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
- halogen,
- C₁-C₄ alkyl,
- halogenated C₁-C₄ alkyl,
- C₁-C₃ alkoxy,
- heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
- halogen,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,
- carboxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkylcarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C₁-C₃ alkyl,
- heterocyclylthio,
- C₁-C₃ alkylsulfonyl,
- mono- or di-C₁-C₃ alkylaminosulfonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,
 - halogenated C₁-C₇ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,

- oxo,
- C₁-C₃ alkylcarbonyloxy,
- C₁-C₃ alkoxycarbonyl,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by carbocyclic aryl,
- C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - heterocyclyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by C₁-C₃ alkyl,
- mono- or di-C₁-C₃ alkylamino,
- C₁-C₄ alkylcarbonylamino,
- C₁-C₃ alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
- heterocyclylthio,
- heterocyclylthio substituted by C₁-C₃ alkyl,
- C₁-C₃ alkylsulfonyl,
- carbocyclic arylsulfonyl,
- carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
- C₁-C₃ alkoxycarbonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl;

Y is -(CH₂)_m, m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9*H*-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, indanyl, or indenyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolo[2,3-*c*]pyridyl, 1*H*-pyrrolyl, 2,2',5',2''-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 3,4-dihydro-2*H*-benzo[*b*][1,4]dioxepinyl, 4*H*-benzo[1,3]dioxinyl, 4*H*-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[*b*]thienyl, benzofuryl, benzothiazolyl, furyl, imidazo[2,1-*b*]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperazyl, piperidyl, pyrazolo[5,1-*b*]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, or thiolanyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

11. A compound according to claim 10, wherein

R₁ represents

(i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- methoxy,
- methoxy substituted by carbocyclic aryl,

- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-C₁-C₂ alkylamino substituted by cyano,
- mono- or di-C₁-C₂ alkylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - heterocyclyl substituted by carbocyclic aryl,
- (ii) C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
- (iii) C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₉ alkyl,
 - halogenated C₁-C₉ alkyl,

- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
- halogen,
- halogenated carbocyclic aryl,
- propenyloxy,
- methylamino,
- di-C₁-C₂ alkylamino,
- di-C₁-C₂ alkylamino substituted by cyano,
- methylthio,
- halogenated methylthio,

(vii) heterocyclyl,

or heterocyclyl substituted by substituent(s) independently selected from

- halogen,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by hydroxy,
- C₁-C₄ alkyl substituted by carbocyclic aryl,
- methoxy,
- C₁-C₂ alkoxy carbonyl,
- carbocyclic arylthio substituted by methoxycarbonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- halogenated methyl,
- heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9*H*-fluorenyl, acenaphthyl, or anthraquinonyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,2',5',2''-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[*b*]thienyl, benzofuryl,

benzothiazolyl, furyl, imidazolyl, isoxazolyl, oxolanyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, 2*H*-benzopyranyl, 4*H*-benzo[1,3]dioxinyl, azetidiny, imidazo[2,1-b]thiazolyl, morpholinyl, or 2,3-dihydro-benzofuryl;

halogen is fluoro, chloro, bromo, or iodo;
or a salt thereof.

12. A compound according to claim 11, wherein

R₁ represents

(i) C₁-C₇ alkyl substituted by substituent(s) independently selected from

- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-ethylamino substituted by cyano,
- di-methylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - methoxy,
 - halogenated methoxy,
 - heterocyclyl substituted by carbocyclic aryl,

(ii) C₂-C₇ alkenyl substituted by substituent(s) independently selected from

- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,

- carbocyclic aryl substituted by methoxy,
- (iii) butynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₂ alkyl,
 - halogenated methyl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - halogenated carbocyclic aryl,
 - propenyloxy,
 - di-C₁-C₂ alkylamino,
 - di-C₁-C₂ alkylamino substituted by cyano,
 - methylthio,
 - halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by hydroxy,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - methoxy,
 - ethoxycarbonyl,
 - carbocyclic arylthio substituted by methoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- halogenated methyl,
- heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, **naphthyl**, or biphenyl;

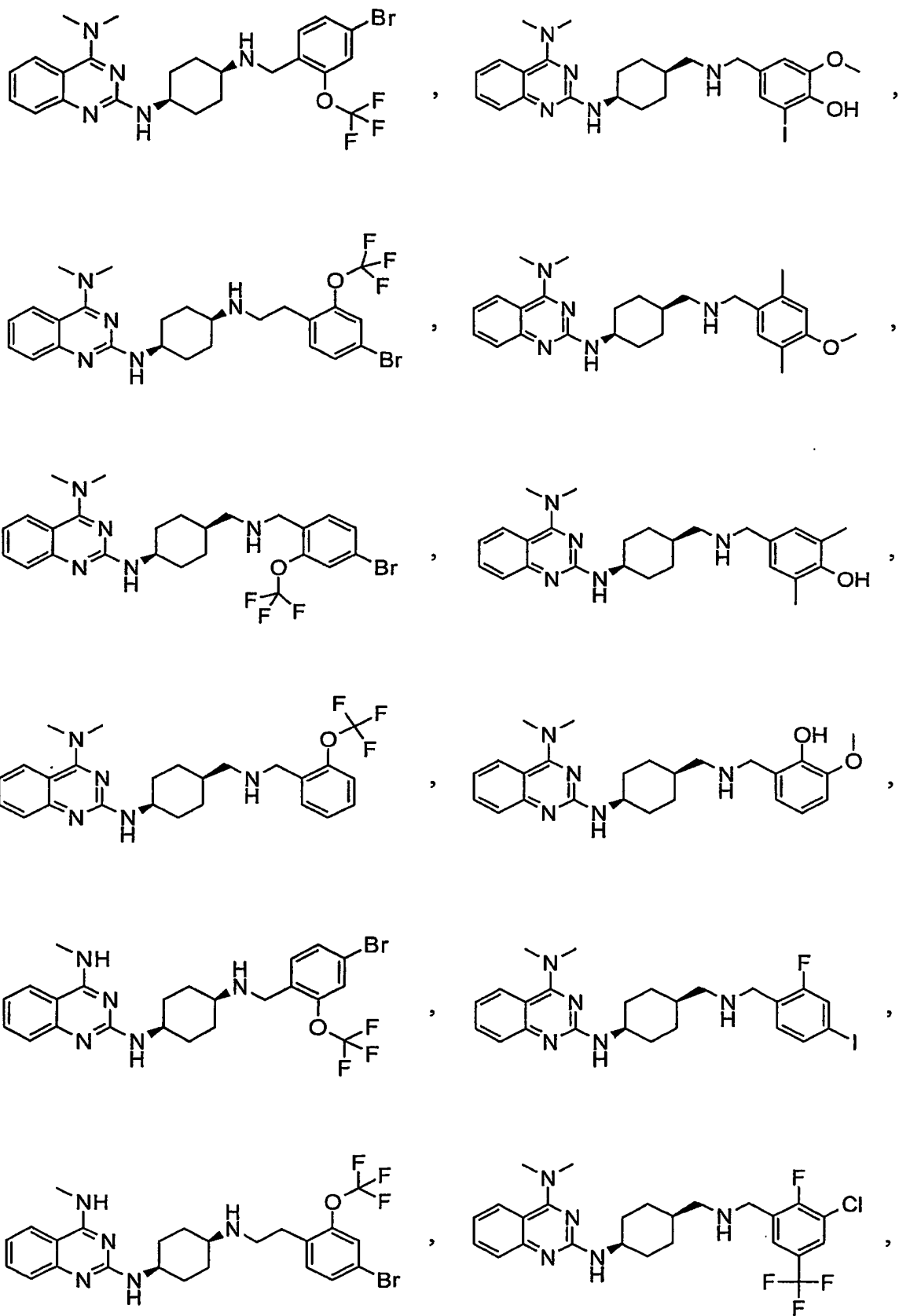
carbocyclyl is acenaphthyl;

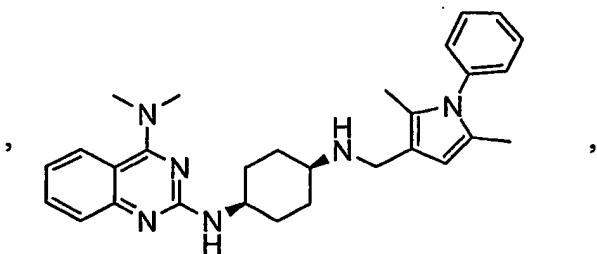
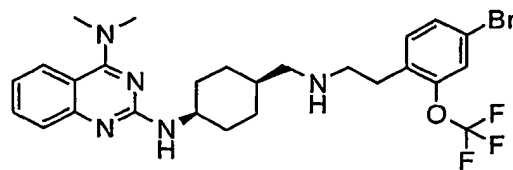
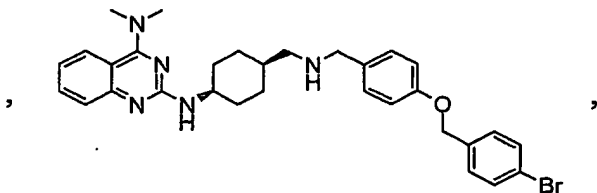
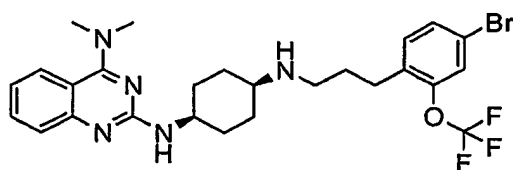
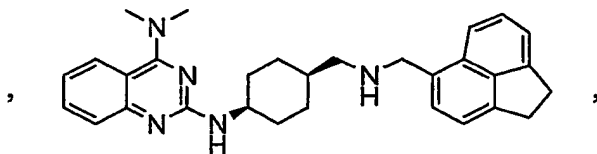
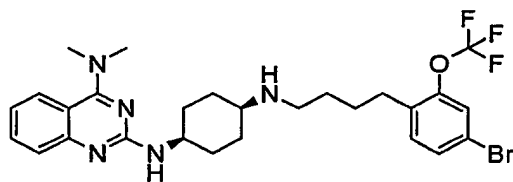
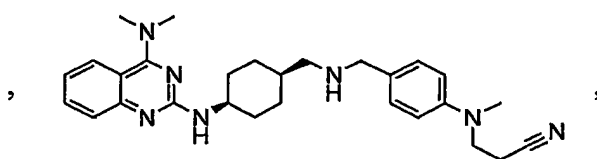
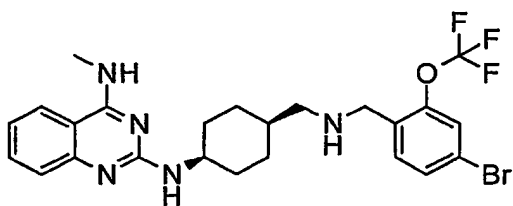
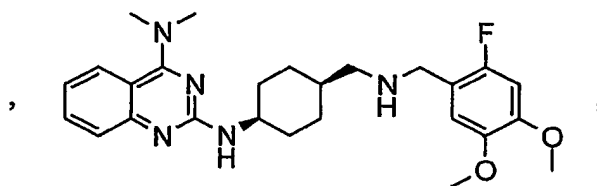
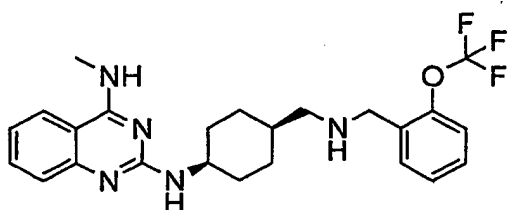
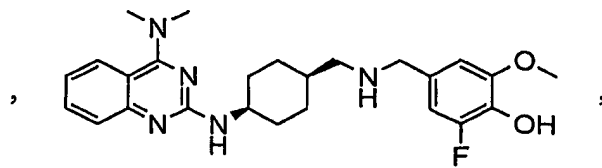
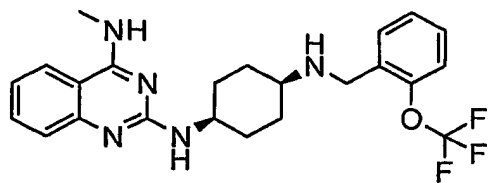
heterocyclyl is 1*H*-indolyl, 1*H*-pyrrolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 9*H*-carbazolyl, benzo[1,3]dioxolyl, furyl, pyrazolyl, thienyl, 4-oxo-benzopyranyl, azetidiny, imidazo[2,1-*b*]thiazolyl, pyridyl, imidazolyl, 2,3-dihydro-benzofuryl, or benzo[*b*]thienyl;

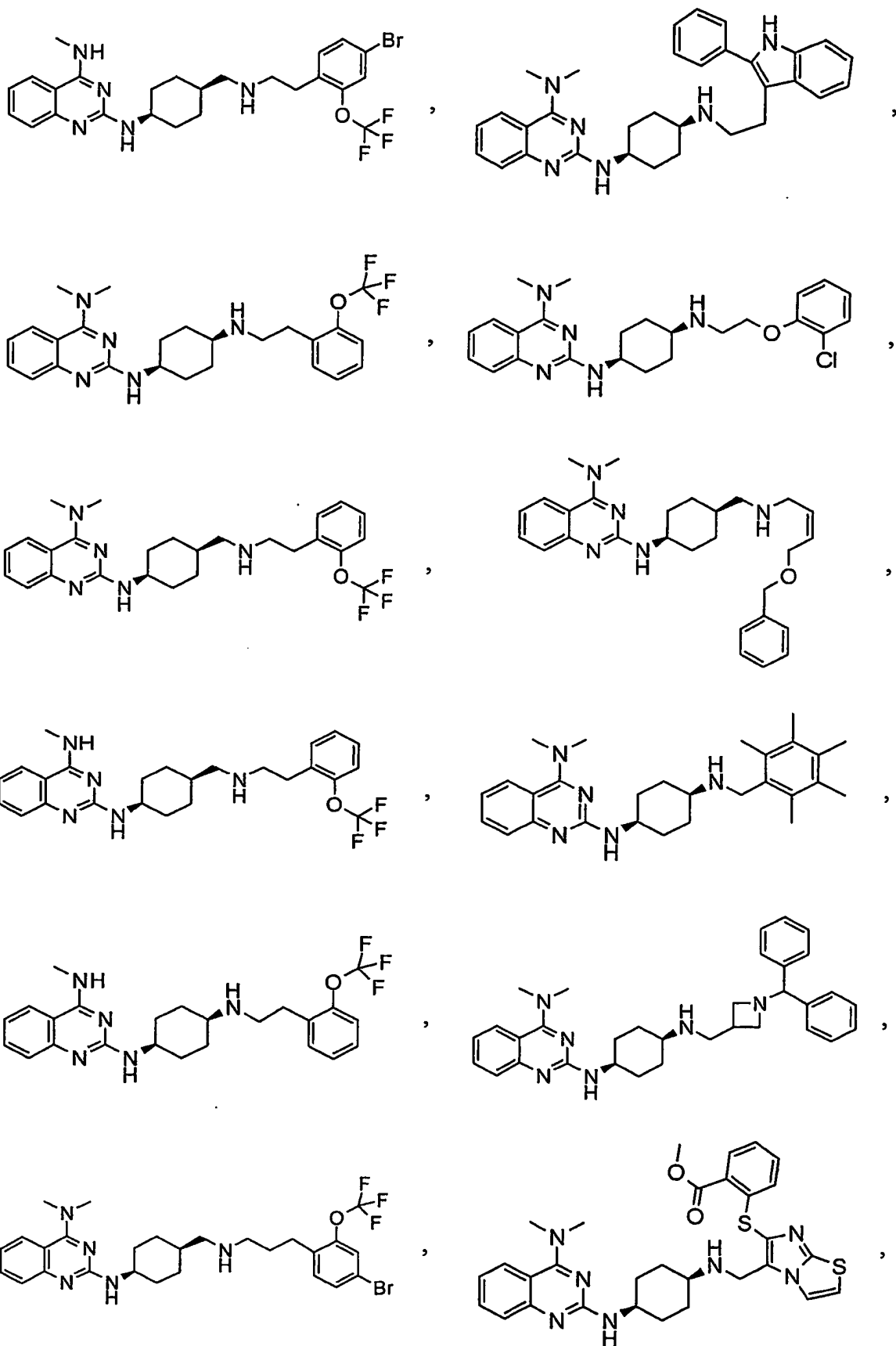
halogen is fluoro, chloro, bromo, or iodo;

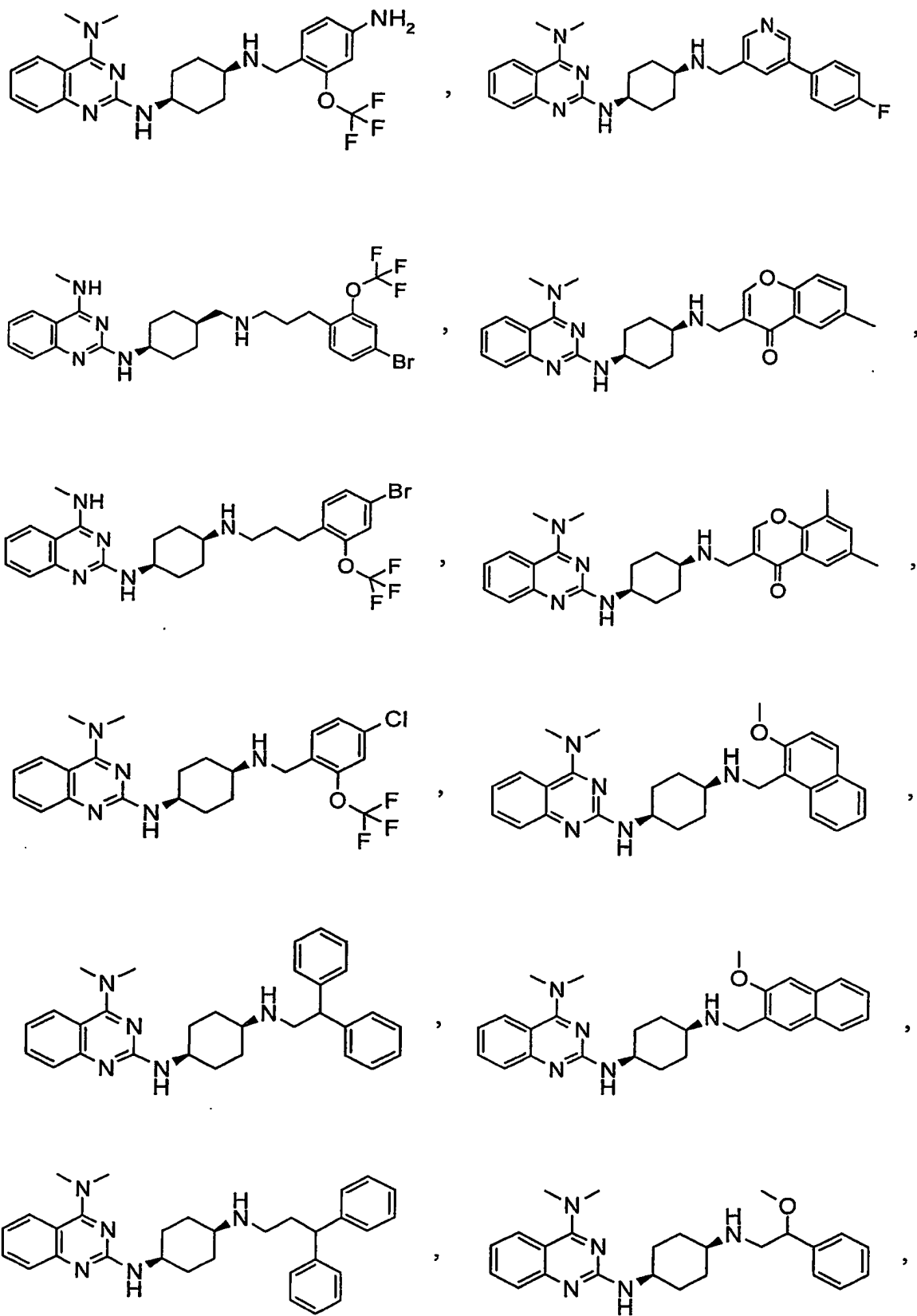
or a salt thereof.

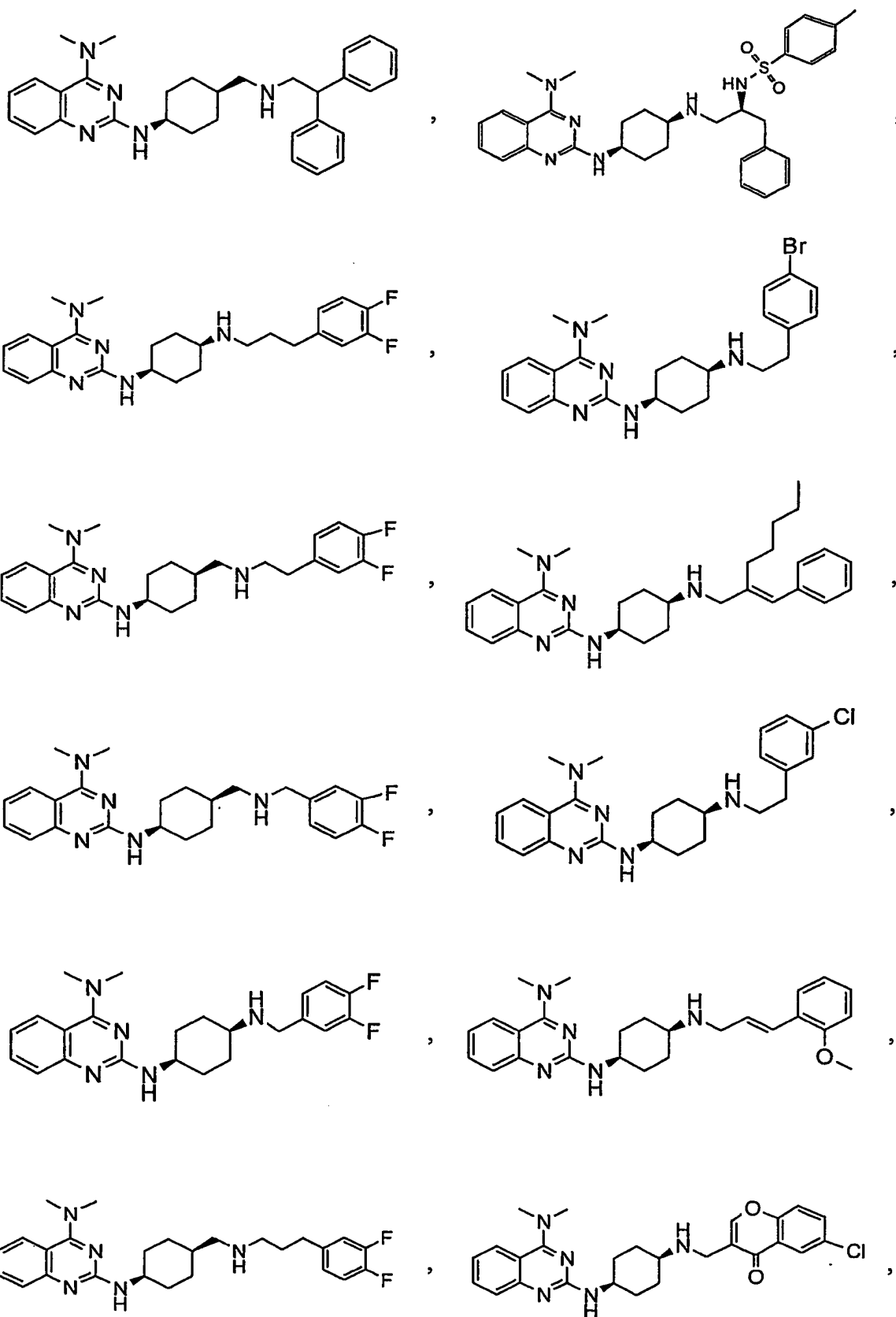
13. A compound according to claim 12 of Formua I selected from the group consisting of

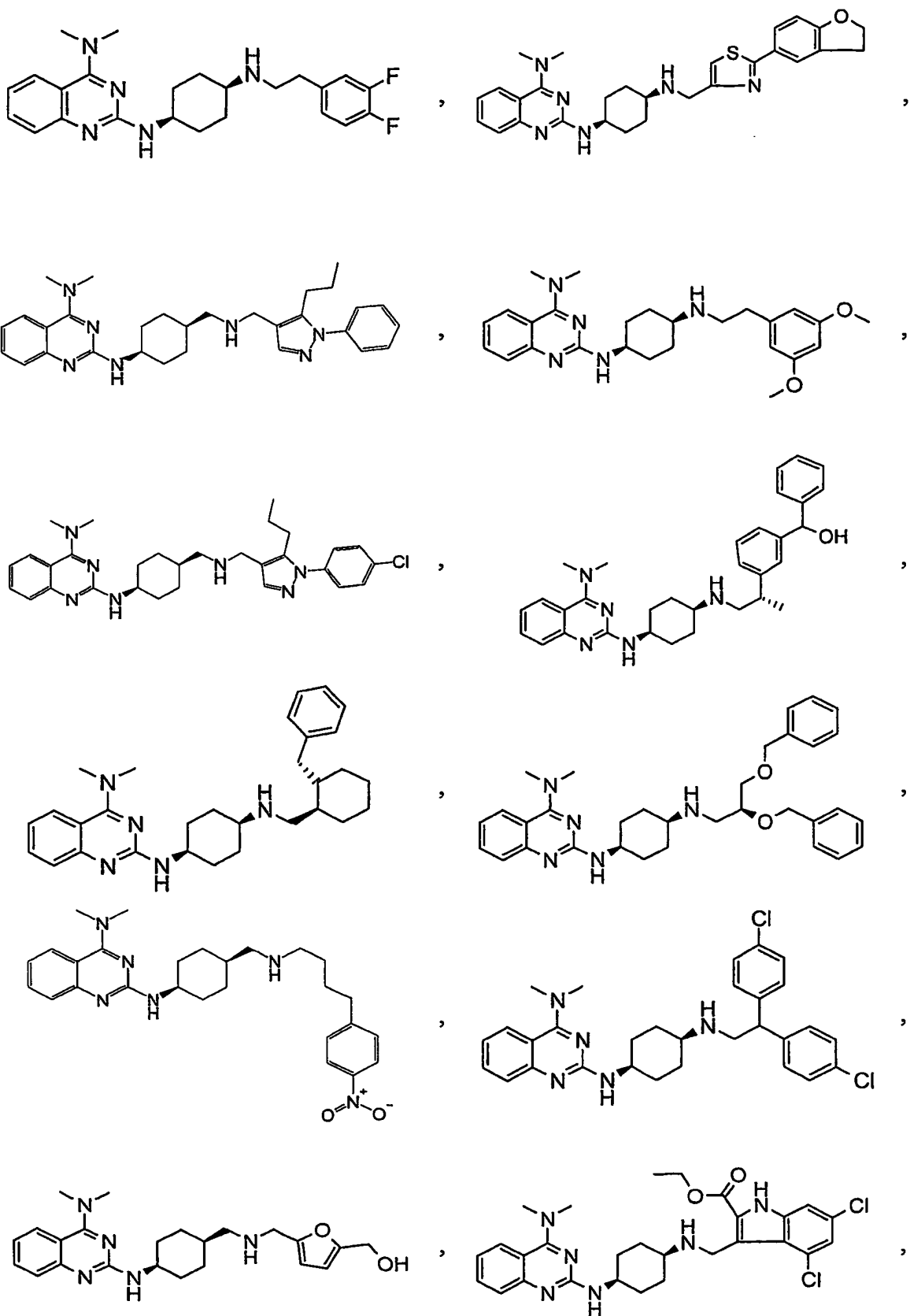


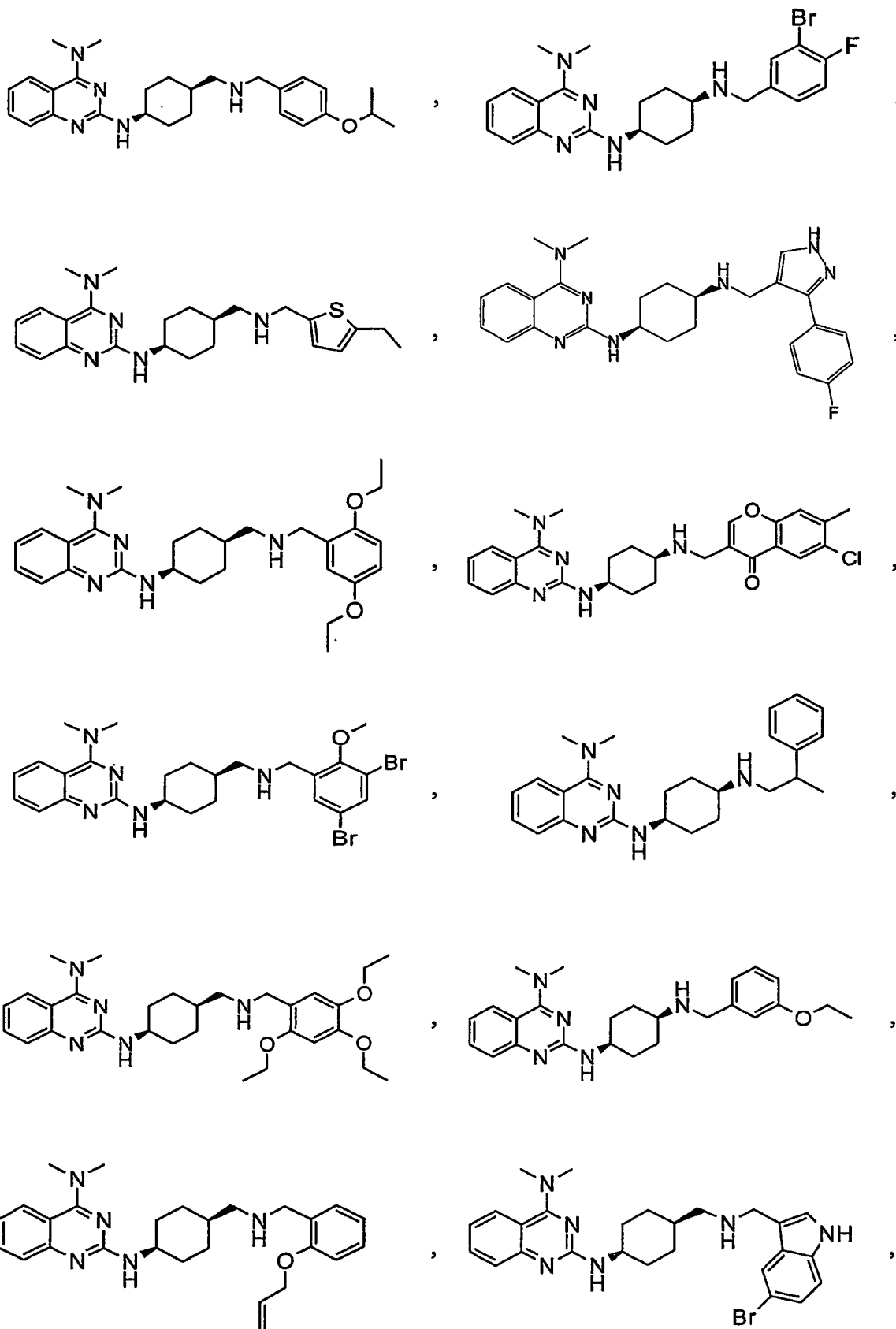


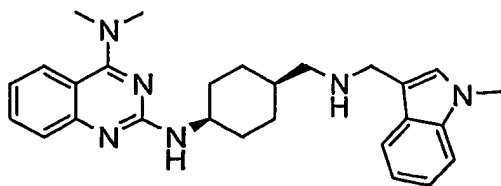




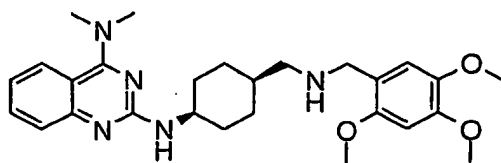




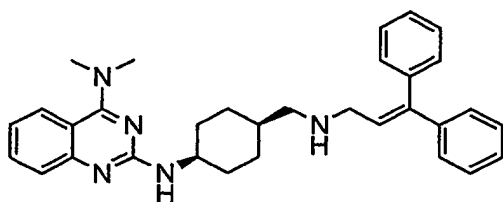




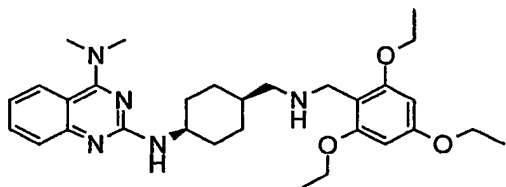
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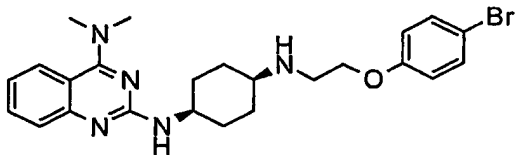
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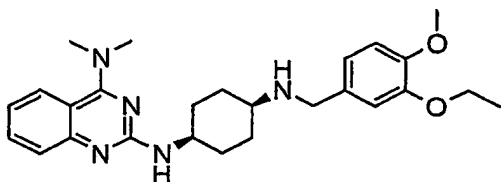
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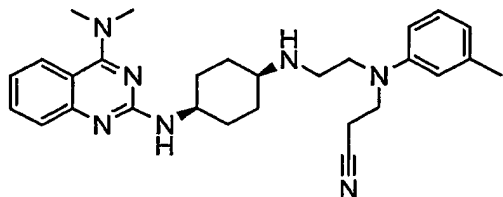
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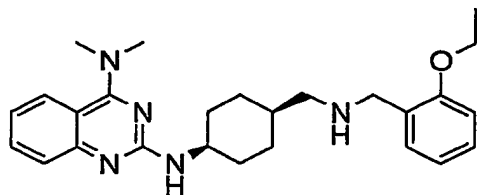
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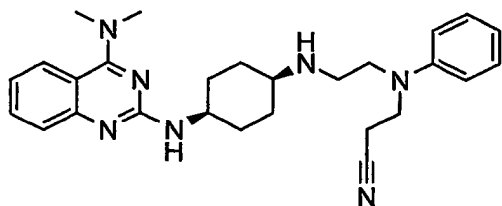
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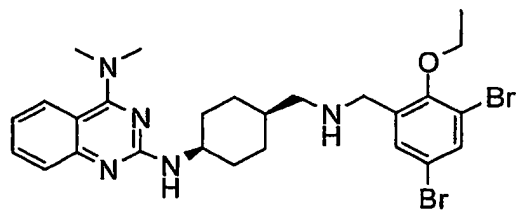
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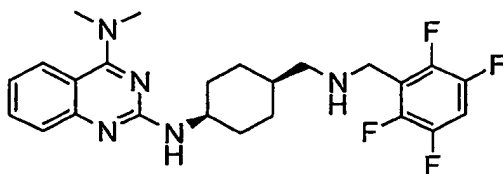
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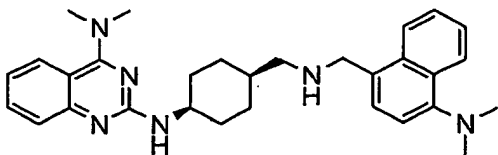
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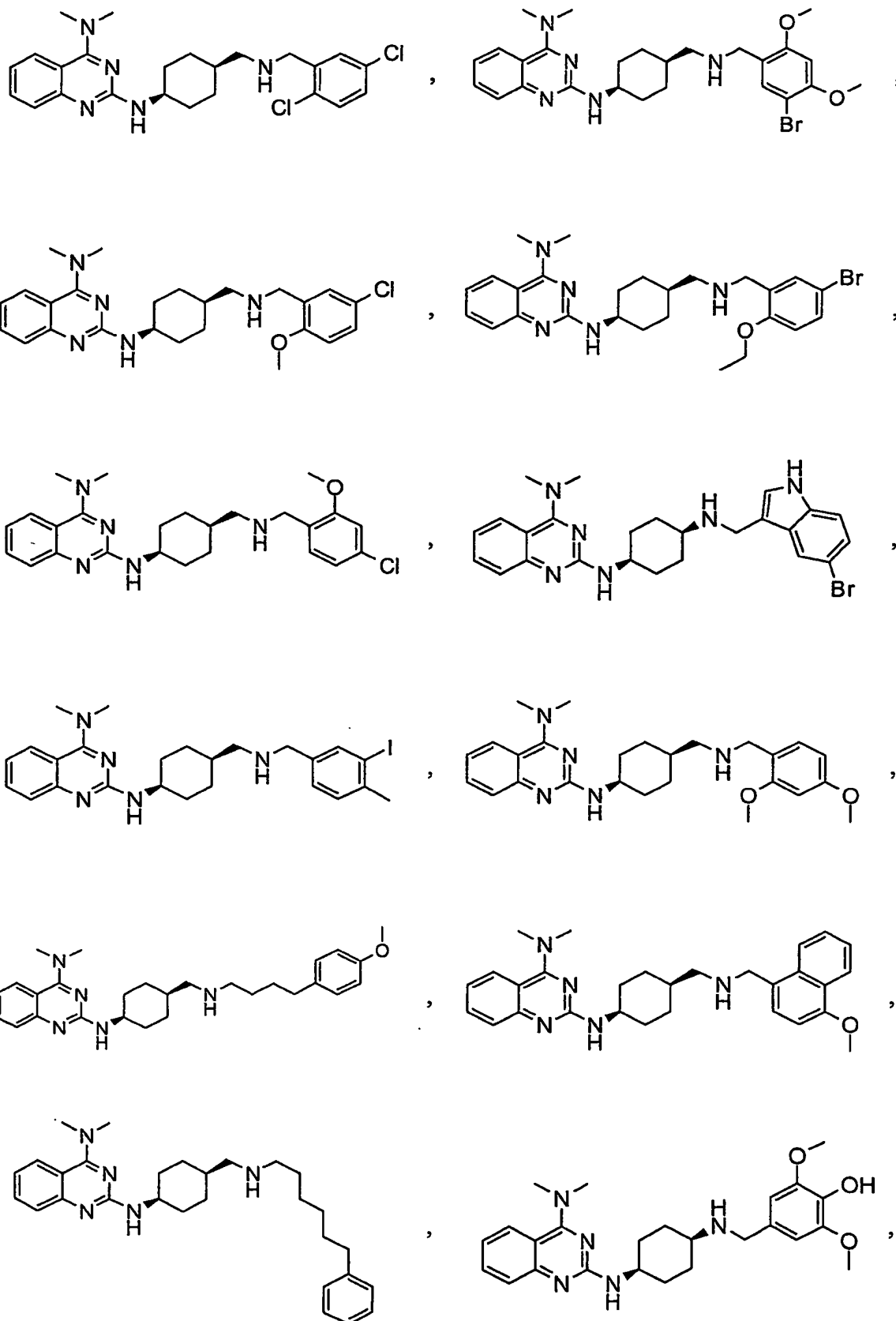
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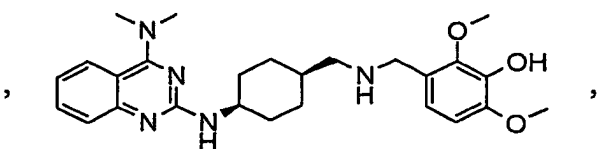
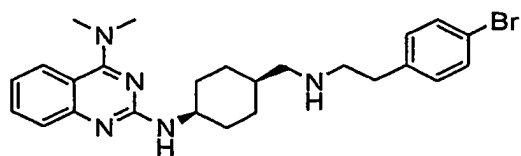
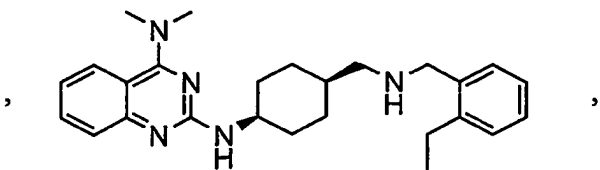
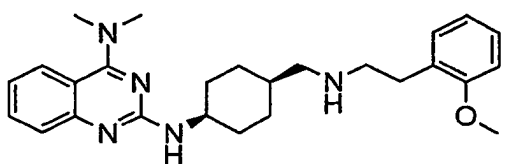
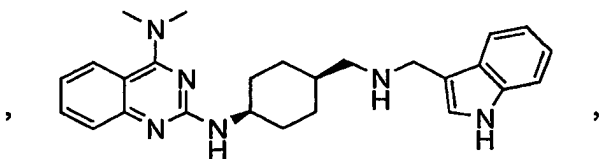
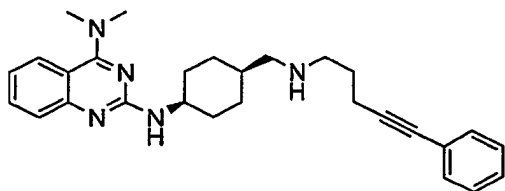
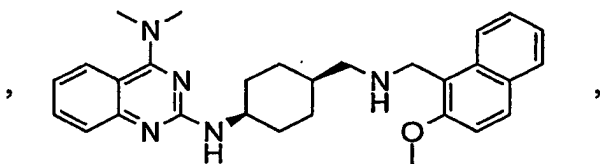
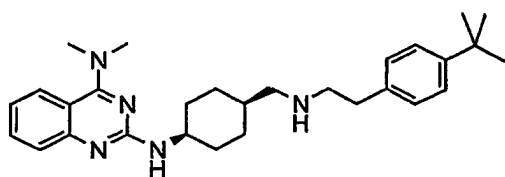
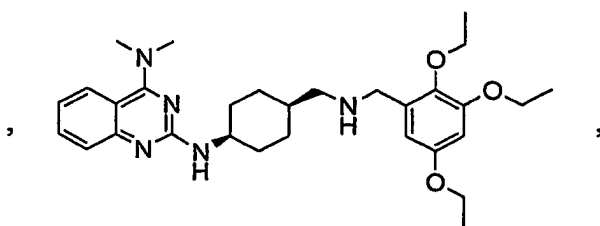
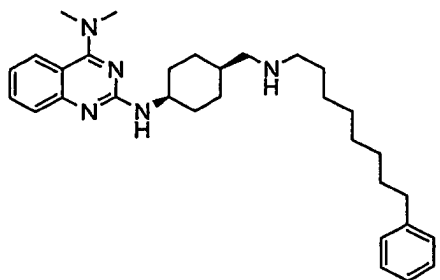
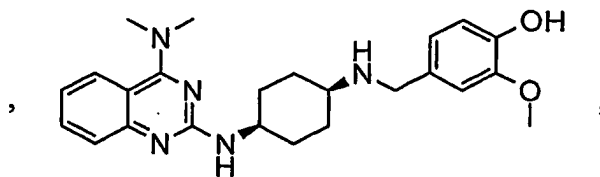
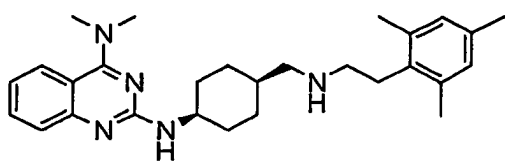


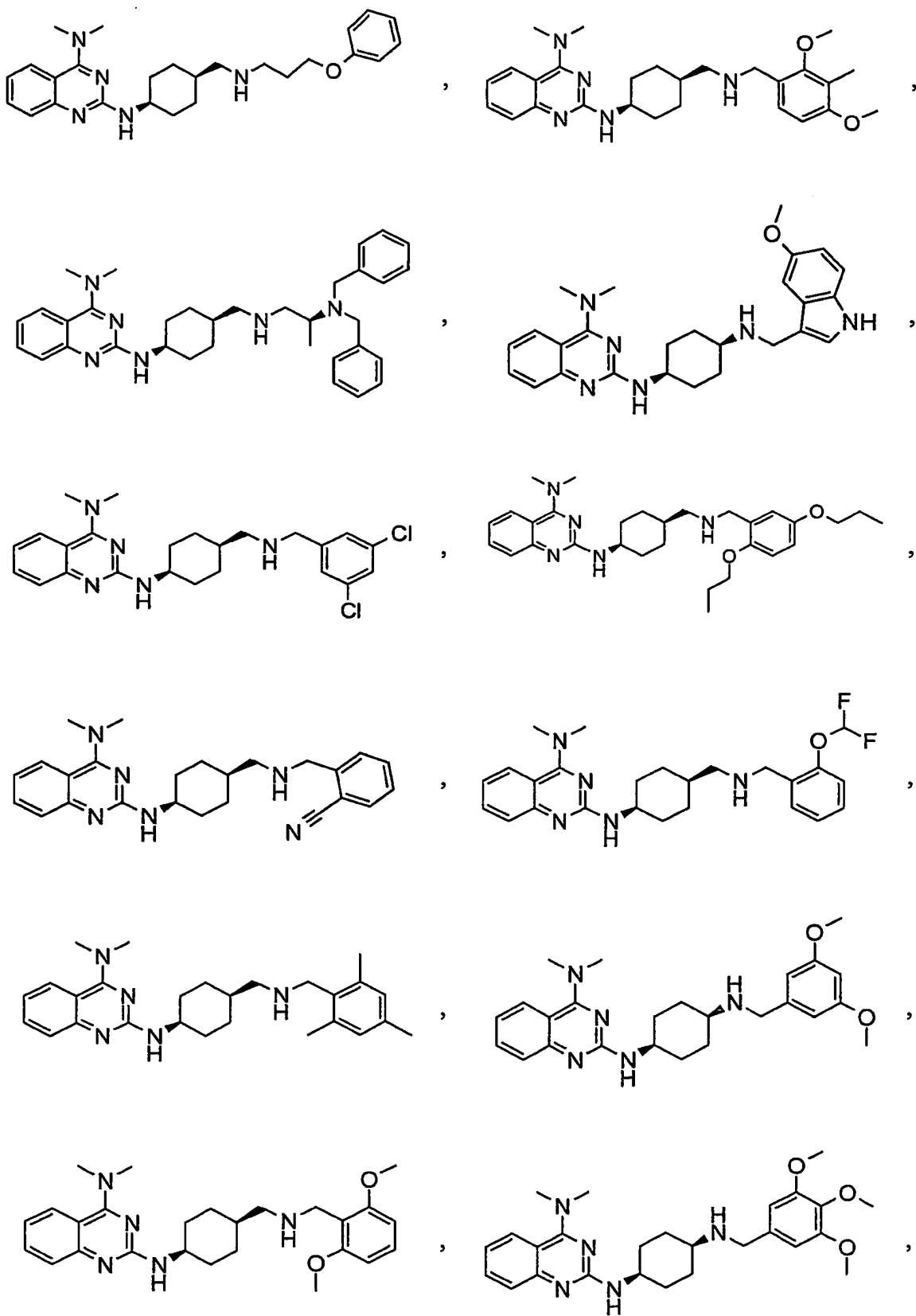
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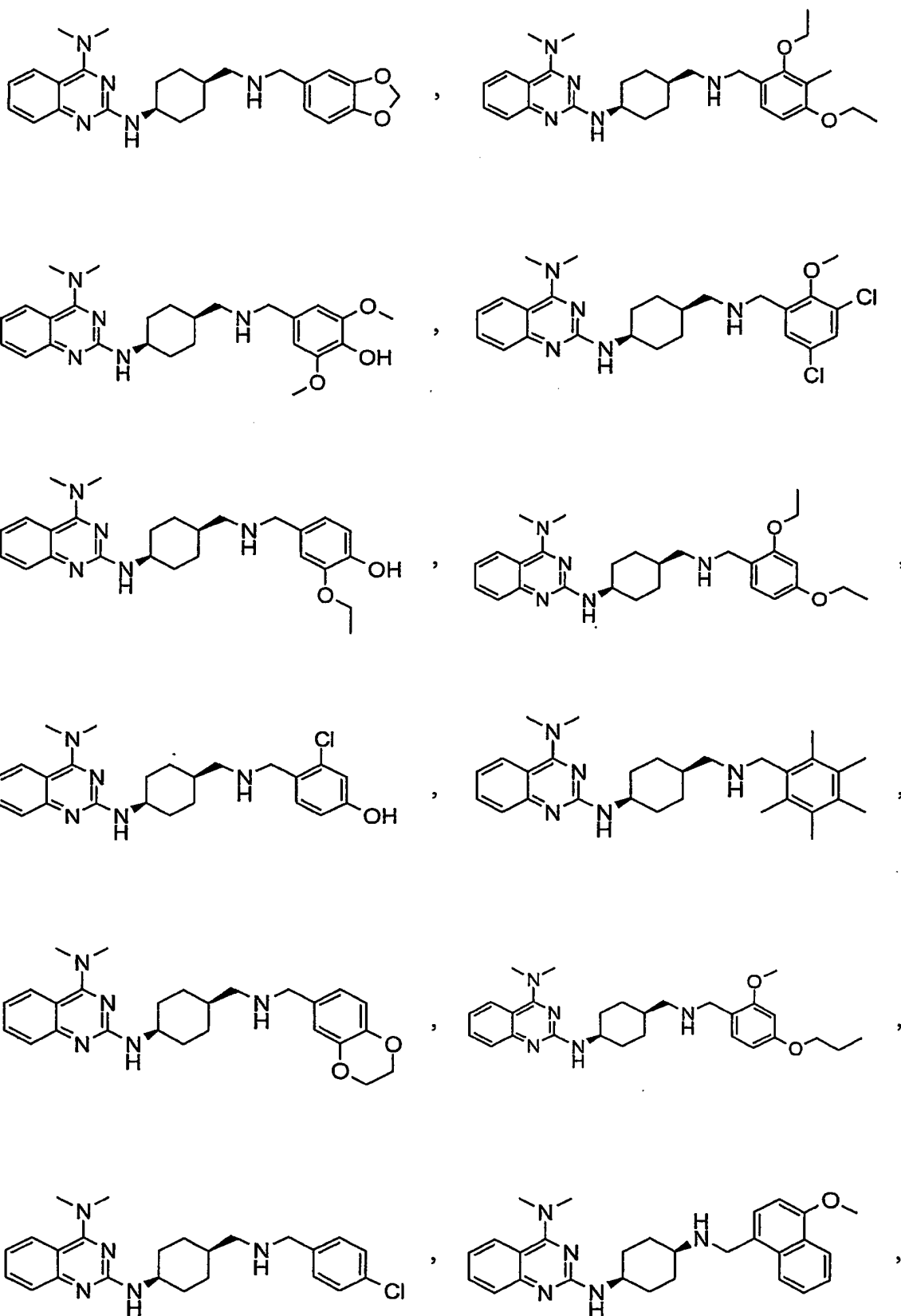


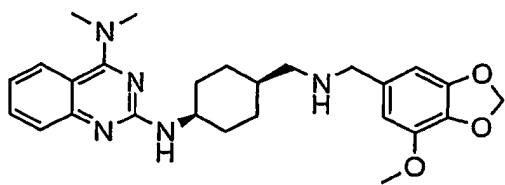
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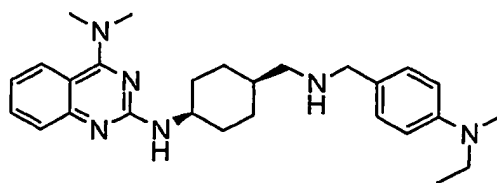




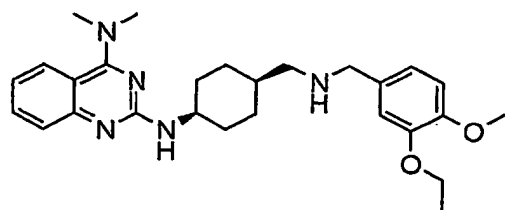




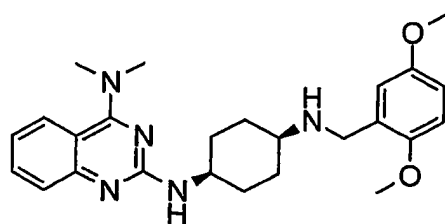
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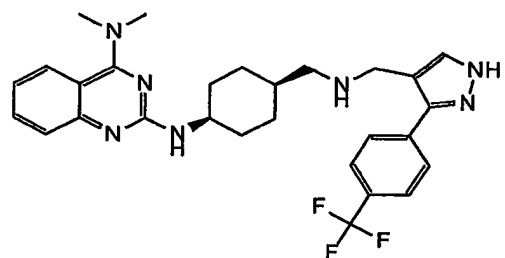
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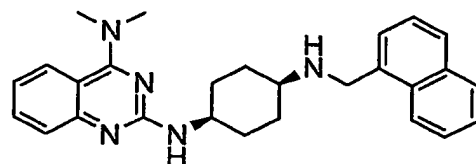
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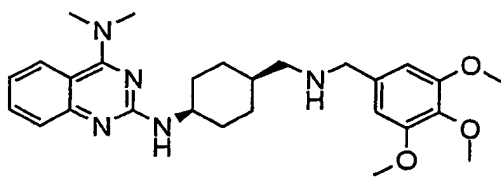
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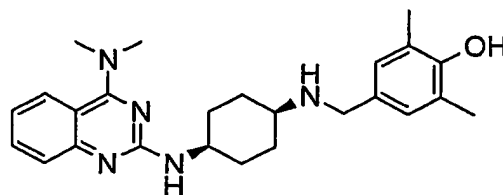
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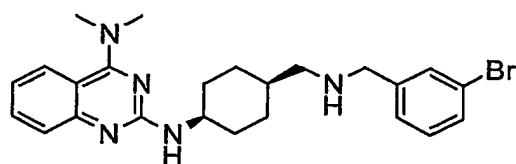
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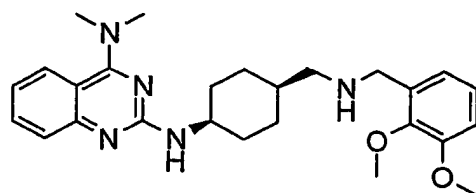
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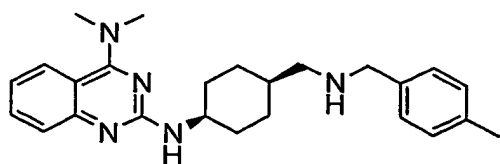
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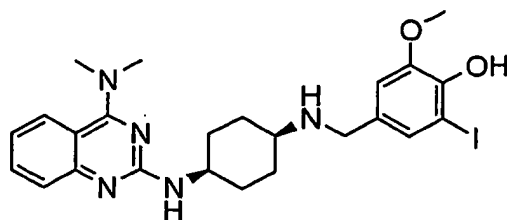
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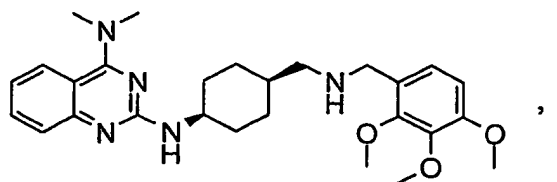
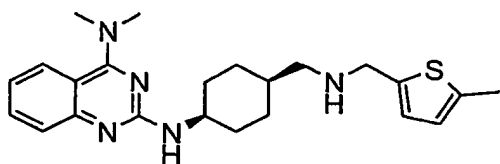
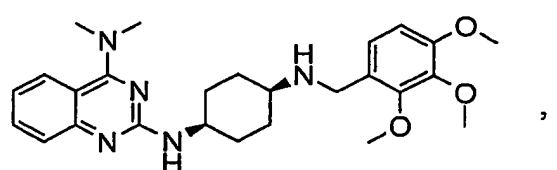
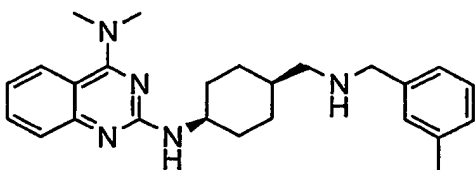
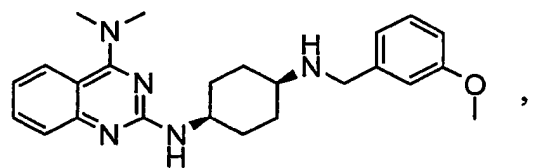
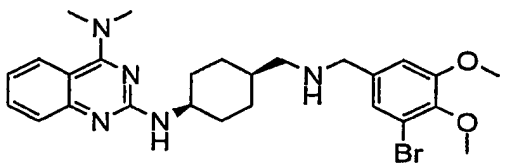
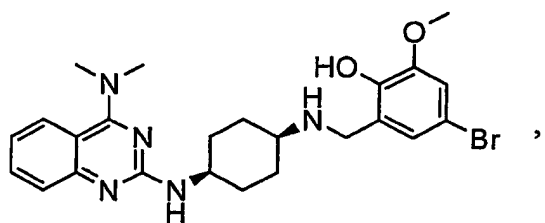
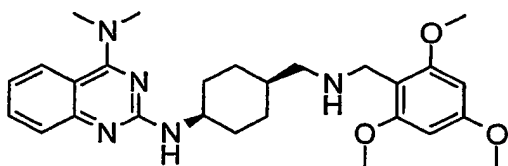
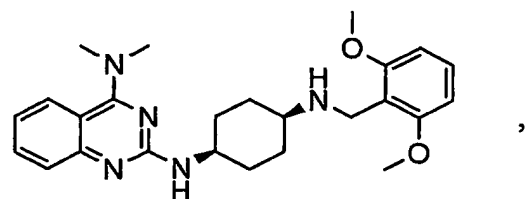
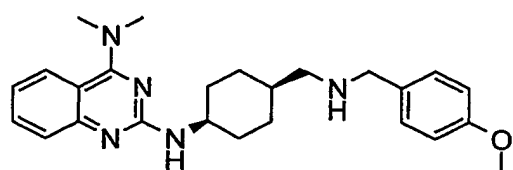
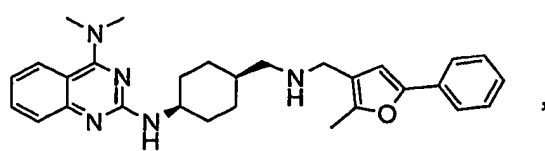
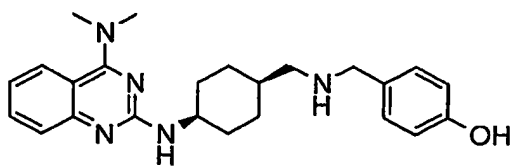
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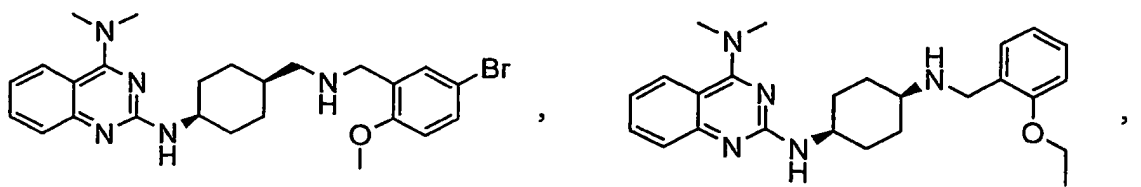
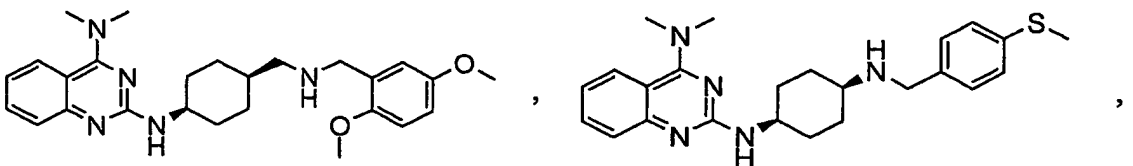
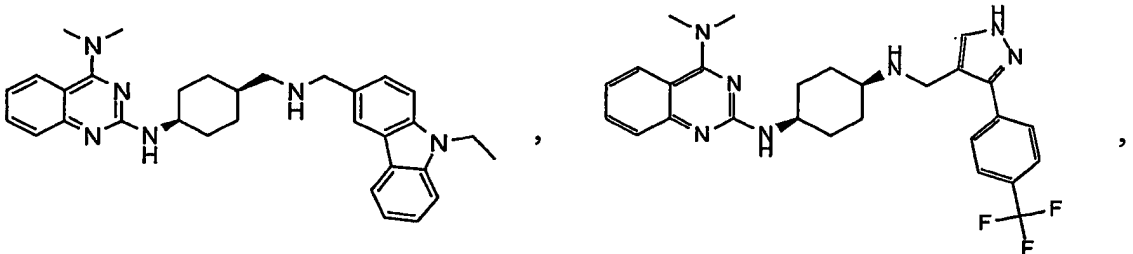
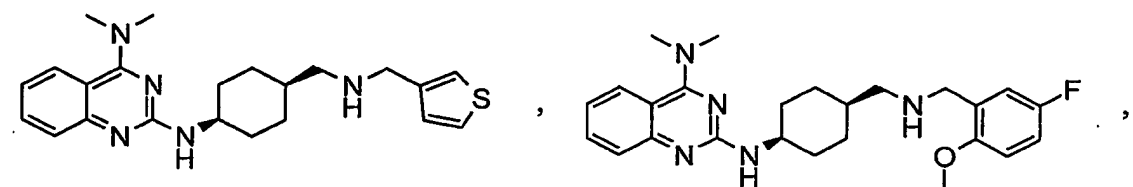
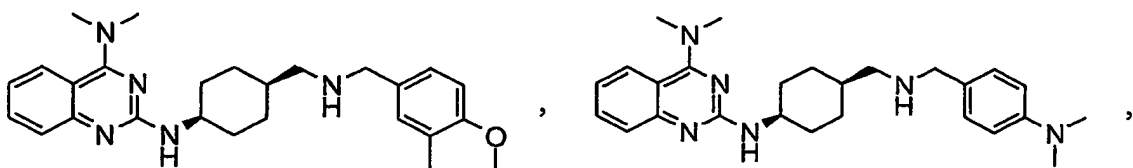
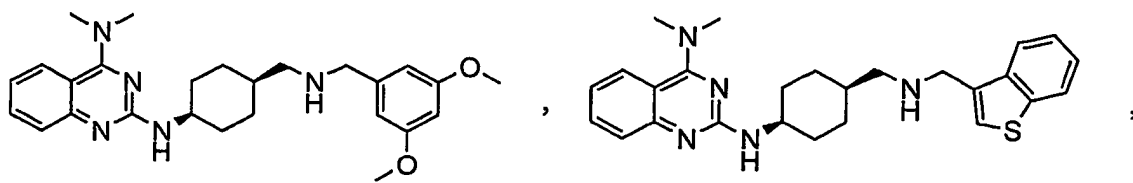


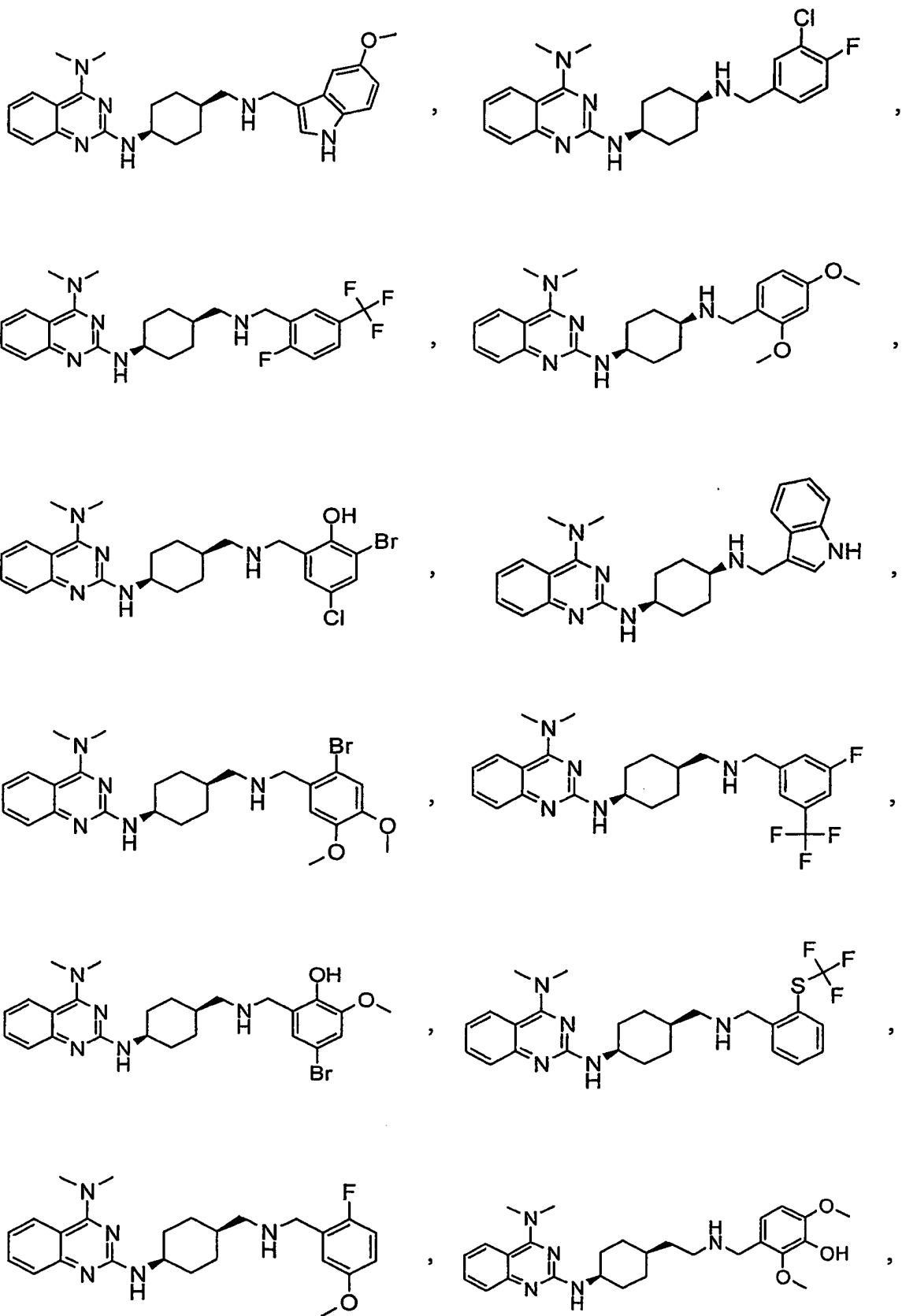
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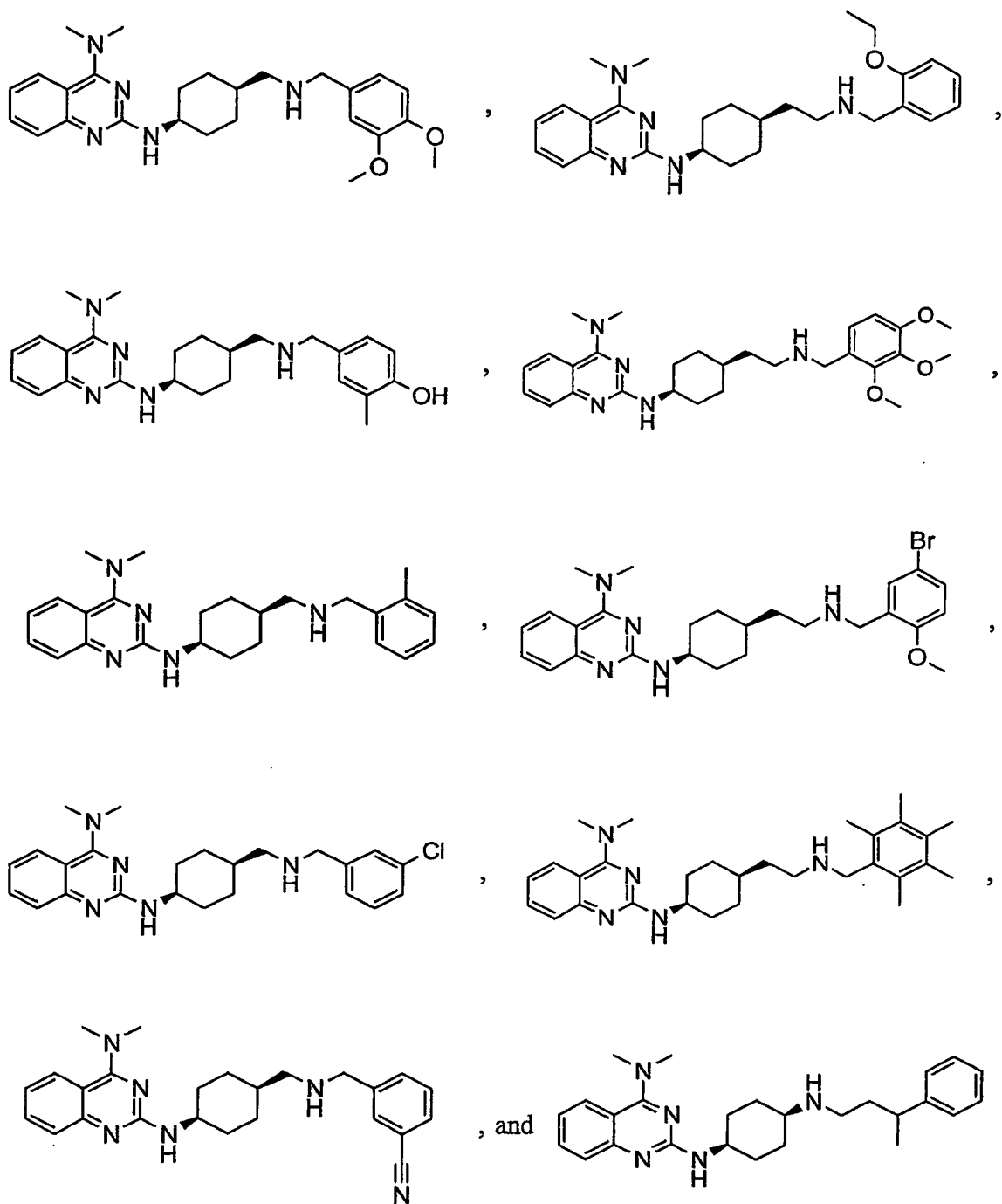


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; or, in case of, a salt thereof.

14. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

•halogen,

•carbocyclyl,

•carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

••C₁-C₃ alkoxy,

••halogenated C₁-C₃ alkoxy,

(ii) C₂-C₃ alkenyl,

C₂-C₃ alkenyl substituted by carbocyclic aryl,

(iii) carbocyclic aryl,

carbocyclic aryl substituted by substituent(s) independently selected from

•halogen,

•cyano,

•nitro,

•C₁-C₅ alkyl,

•C₁-C₅ alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

•C₂-C₃ alkenyl,

•C₁-C₄ alkoxy,

•C₁-C₄ alkoxy substituted by substituent(s) independently selected from

••halogen,

••heterocyclyl,

••halogenated heterocyclyl,

•carbocyclic aryloxy,

- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
- heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₄ alkylamino,
 - C₁-C₃ alkylcarbonylamino,
 - carbocyclic aryl diazo,
 - carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic aryl,
- (iv) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
- C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic arylcarbonylamino,
 - halogenated carbocyclic arylcarbonylamino,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkylcarbonylamino,
 - carbocyclic arylsulfonyl,

- C₁-C₃ alkoxy carbonyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -S(O)₂-;

wherein carbocyclic aryl is phenyl, biphenyl, or naphthyl;

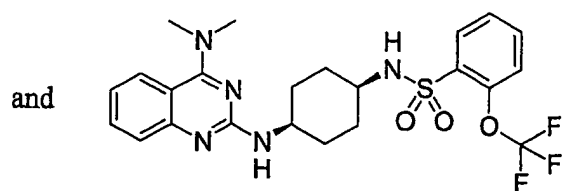
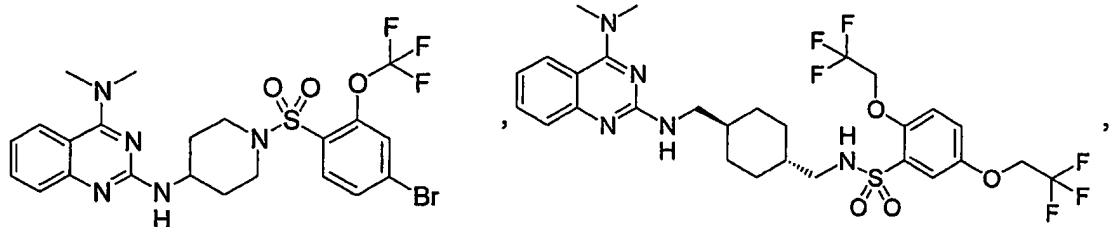
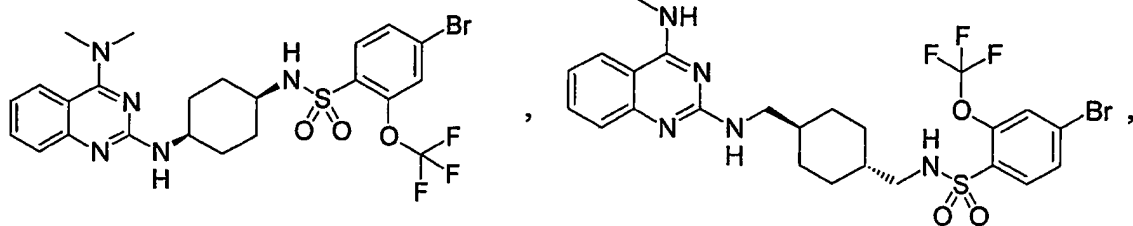
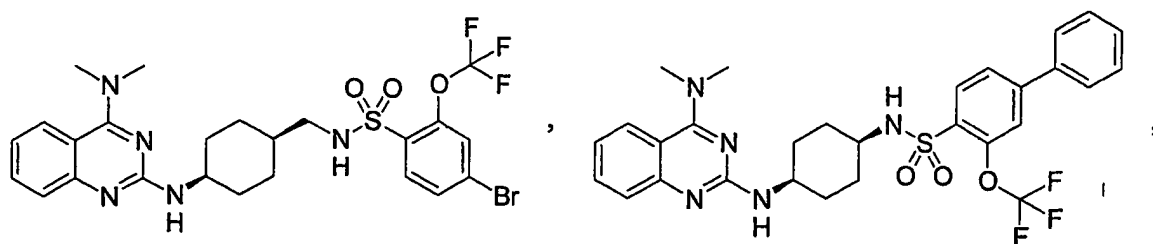
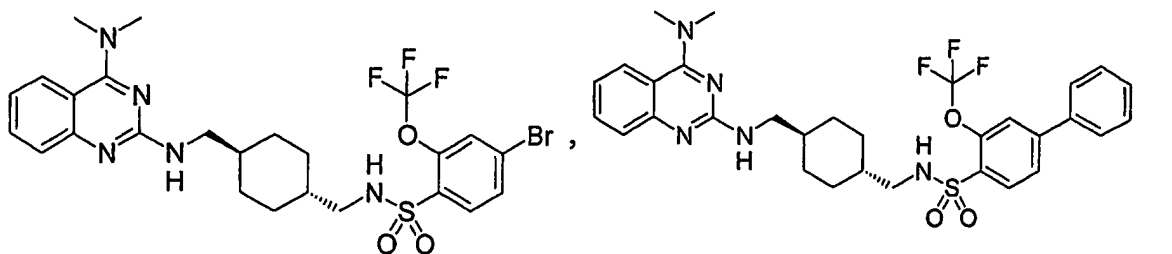
carbocyclyl is 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1*H*-pyrrolyl, benzo[2,1,3]oxadiazolyl, benzo[*b*]thienyl, furyl, imidazolyl, isoxazolyl, pyrazolyl, pyridyl, quinolyl, thiazolyl, or thienyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

15. A compound according to claim 14 of Formula I selected from the group consisting of



; or, in case of, a salt thereof.

16. A compound according to claim 1, wherein Q is Formula II;
R₁ is selected from H, -CO₂^tBu, or -CO₂Bn (Bn is a benzyl group);
R₂ is methylamino or dimethylamino;
L is selected from Formula XX - XXII;
Y is a single bond;
or a salt thereof.

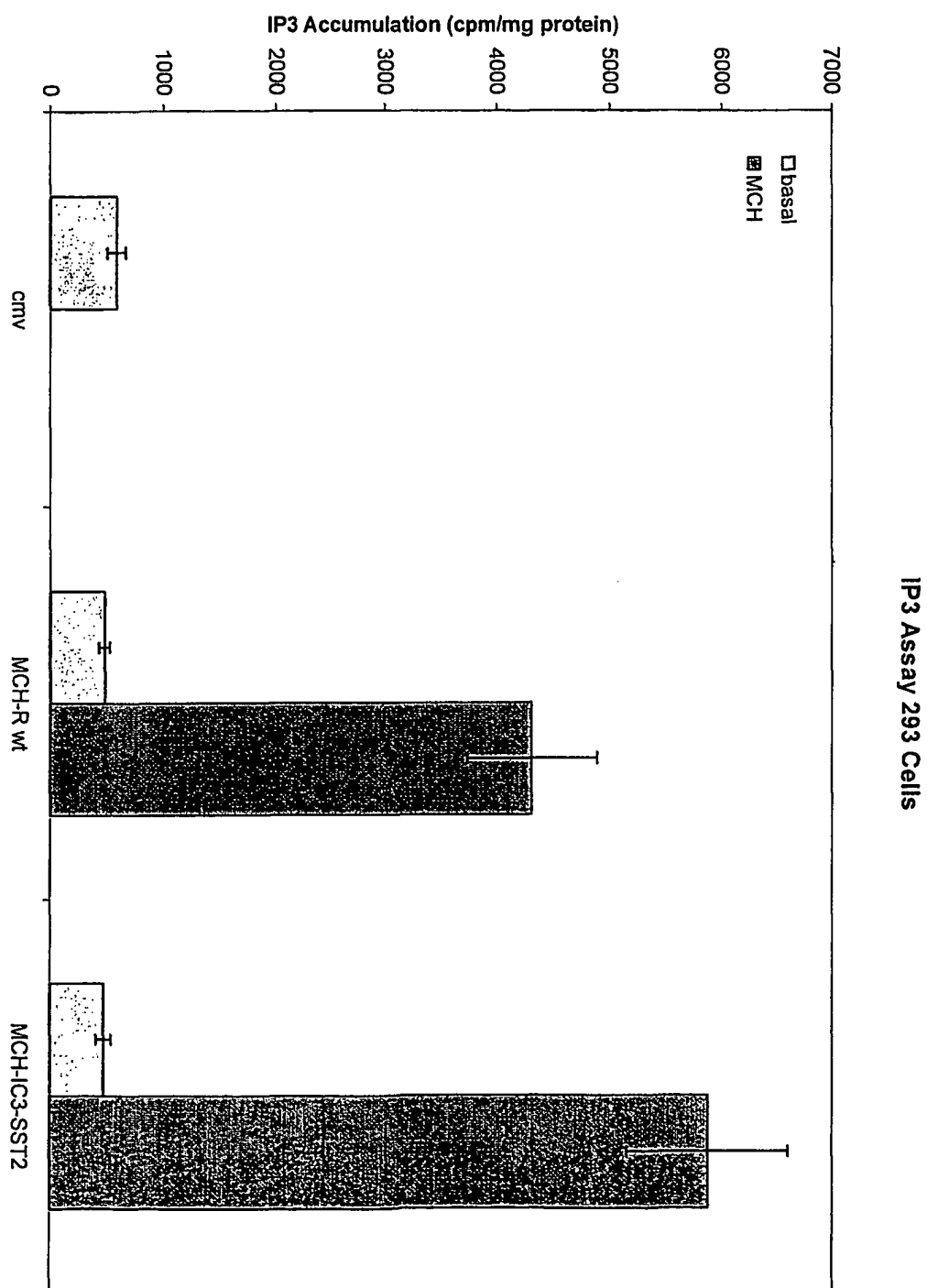
17. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a MCH receptor antagonist.

18. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a compound of claims 1-16.

19. The method of prophylaxis or treatment of obesity, obesity related disorders, anxiety, or depression in mammals in need of such treatment comprising administering to the mammal a therapeutically effective amount of a compound having the composition of any of claims 1-16.

20. A pharmaceutical composition comprising a pharmaceutically acceptable carrier and a therapeutically effective amount of a compound having the composition of any of claims 1-16.

Fig. 1



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<210> 6

<211> 446

<212> PRT

<213> Homo Sapien

<220>

<223> Novel Sequence

<400> 6

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Thr Gly Ser Ile Ser Tyr Ile Asn Ile Ile Met Pro Ser Val Phe Gly
 35          40          45

Thr Ile Cys Leu Leu Gly Ile Ile Gly Asn Ser Thr Val Ile Phe Ala
 50          55          60

Val Val Lys Lys Ser Lys Leu His Trp Cys Asn Asn Val Pro Asp Ile
 65          70          75          80

Phe Ile Ile Asn Leu Ser Val Val Asp Leu Leu Phe Leu Leu Gly Met
 85          90          95

Pro Phe Met Ile His Gln Leu Met Gly Asn Gly Val Trp His Phe Gly
100          105          110

Glu Thr Met Cys Thr Leu Ile Thr Ala Met Asp Ala Asn Ser Gln Phe
115          120          125

Thr Ser Thr Tyr Ile Leu Thr Ala Met Ala Ile Asp Arg Tyr Leu Ala
130          135          140

Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala
145          150          155          160

Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr
165          170          175

Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val
180          185          190

Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe
195          200          205

Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
210          215          220

Thr Ala Ala Tyr Val Arg Ile Leu Gln Lys Val Lys Ser Ser Gly Ile
225          230          235          240

Arg Val Gly Ser Ser Lys Arg Lys Lys Ser Glu Lys Lys Val Thr Arg
245          250          255

Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
260          265          270

Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
275          280          285

Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser

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290	295	300
Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys		
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Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala		
	325	330 335
Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly		
	340	345 350
Thr Tyr Phe Pro Cys His Pro Ala His Leu Gln Val Arg Ala Pro Gln		
	355	360 365
His Ala Thr Gly Arg Asp Ala Glu Lys Asn Pro Arg Pro Leu Gly Lys		
	370	375 380
Cys Arg Lys Ala Gly Leu Gly Val Val Ala Met Lys Ile His Ser Met		
385	390	395 400
Gly Ser His Val Ala Gly Glu Ala Trp Ser Gln Val Trp Gly Phe Gln		
	405	410 415
Ile Ser Glu Ile Pro Trp Gly Ser Arg Met Arg Pro Leu Asp Arg Thr		
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<210> 8

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<213> Artificial

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<210> 11

<211> 2133

<212> DNA

<213> Homo Sapien

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<210> 12

<211> 709

<212> PRT

<213> Homo Sapien

<400> 12

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			20					25					30		
Thr	Gly	Ser	Ile	Ser	Tyr	Ile	Asn	Ile	Ile	Met	Pro	Ser	Val	Phe	Gly
		35					40					45			
Thr	Ile	Cys	Leu	Leu	Gly	Ile	Ile	Gly	Asn	Ser	Thr	Val	Ile	Phe	Ala
	50					55					60				
Val	Val	Lys	Lys	Ser	Lys	Leu	His	Trp	Cys	Asn	Asn	Val	Pro	Asp	Ile
	65				70					75					80
Phe	Ile	Ile	Asn	Leu	Ser	Val	Val	Asp	Leu	Leu	Phe	Leu	Leu	Gly	Met
			85						90					95	
Pro	Phe	Met	Ile	His	Gln	Leu	Met	Gly	Asn	Gly	Val	Trp	His	Phe	Gly
			100					105					110		
Glu	Thr	Met	Cys	Thr	Leu	Ile	Thr	Ala	Met	Asp	Ala	Asn	Ser	Gln	Phe
		115					120					125			
Thr	Ser	Thr	Tyr	Ile	Leu	Thr	Ala	Met	Ala	Ile	Asp	Arg	Tyr	Leu	Ala
	130					135					140				
Thr	Val	His	Pro	Ile	Ser	Ser	Thr	Lys	Phe	Arg	Lys	Pro	Ser	Val	Ala
145					150				155						160
Thr	Leu	Val	Ile	Cys	Leu	Leu	Trp	Ala	Leu	Ser	Phe	Ile	Ser	Ile	Thr
			165					170					175		
Pro	Val	Trp	Leu	Tyr	Ala	Arg	Leu	Ile	Pro	Phe	Pro	Gly	Gly	Ala	Val
			180				185						190		
Gly	Cys	Gly	Ile	Arg	Leu	Pro	Asn	Pro	Asp	Thr	Asp	Leu	Tyr	Trp	Phe
	195						200					205			

Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
 210 215 220
 Thr Ala Ala Tyr Val Arg Ile Leu Gln Arg Met Thr Ser Ser Val Ala
 225 230 235 240
 Pro Ala Ser Gln Arg Ser Ile Arg Leu Arg Thr Lys Arg Val Thr Arg
 245 250 255
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
 260 265 270
 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
 275 280 285
 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser
 290 295 300
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys
 305 310 315 320
 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala
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 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly
 340 345 350
 Thr Ser Arg Met Gly Cys Thr Leu Ser Ala Glu Asp Lys Ala Ala Val
 355 360 365
 Glu Arg Ser Lys Met Ile Asp Arg Asn Leu Arg Glu Asp Gly Glu Lys
 370 375 380
 Ala Ala Arg Glu Val Lys Leu Leu Leu Leu Gly Ala Gly Glu Ser Gly
 385 390 395 400
 Lys Ser Thr Ile Val Lys Gln Met Lys Ile Ile His Glu Ala Gly Tyr
 405 410 415
 Ser Glu Glu Glu Cys Lys Gln Tyr Lys Ala Val Val Tyr Ser Asn Thr
 420 425 430
 Ile Gln Ser Ile Ile Ala Ile Ile Arg Ala Met Gly Arg Leu Lys Ile
 435 440 445
 Asp Phe Gly Asp Ala Ala Arg Ala Asp Asp Ala Arg Gln Leu Phe Val
 450 455 460
 Leu Ala Gly Ala Ala Glu Glu Gly Phe Met Thr Ala Glu Leu Ala Gly
 465 470 475 480
 Val Ile Lys Arg Leu Trp Lys Asp Ser Gly Val Gln Ala Cys Phe Asn
 485 490 495
 Arg Ser Arg Glu Tyr Gln Leu Asn Asp Ser Ala Ala Tyr Tyr Leu Asn
 500 505 510

Asp Leu Asp Arg Ile Ala Gln Pro Asn Tyr Ile Pro Thr Gln Gln Asp
 515 520 525
 Val Leu Arg Thr Arg Val Lys Thr Thr Gly Ile Val Glu Thr His Phe
 530 535 540
 Thr Phe Lys Asp Leu His Phe Lys Met Phe Asp Val Gly Gly Gln Arg
 545 550 555 560
 Ser Glu Arg Lys Lys Trp Ile His Cys Phe Glu Gly Val Thr Ala Ile
 565 570 575
 Ile Phe Cys Val Ala Leu Ser Asp Tyr Asp Leu Val Leu Ala Glu Asp
 580 585 590
 Glu Glu Met Asn Arg Met His Glu Ser Met Lys Leu Phe Asp Ser Ile
 595 600 605
 Cys Asn Asn Lys Trp Phe Thr Asp Thr Ser Ile Ile Leu Phe Leu Asn
 610 615 620
 Lys Lys Asp Leu Phe Glu Glu Lys Ile Lys Lys Ser Pro Leu Thr Ile
 625 630 635 640
 Cys Tyr Pro Glu Tyr Ala Gly Ser Asn Thr Tyr Glu Glu Ala Ala Ala
 645 650 655
 Tyr Ile Gln Cys Gln Phe Glu Asp Leu Asn Lys Arg Lys Asp Thr Lys
 660 665 670
 Glu Ile Tyr Thr His Phe Thr Cys Ala Thr Asp Thr Lys Asn Val Gln
 675 680 685
 Phe Val Phe Asp Ala Val Thr Asp Val Ile Ile Lys Asn Asn Leu Lys
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 Asp Cys Gly Leu Phe
 705